Introduction to Python
Part 1

v0.6.2

Research Computing Services
Information Services & Technology

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RCS Team and Expertise

- Our Team
  - Scientific Programmers
  - Systems Administrators
  - Graphics/Visualization Specialists
  - Account/Project Managers
  - Special Initiatives (Grants)
- Maintains and administers the Shared Computing Cluster
  - Located in Holyoke, MA
  - ~19,000 CPUs running Linux

- Consulting Focus:
  - Bioinformatics
  - Data Analysis / Statistics
  - Molecular modeling
  - Geographic Information Systems
  - Scientific / Engineering Simulation
  - Visualization

- CONTACT US: help@scc.bu.edu

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Getting Started

- The downloads for the Python tutorials are located at:

  http://rcs.bu.edu/examples/python/tutorials/

- That link has two files for downloading.
  - One is a copy of this presentation.
  - The other, *rcs_py_tutorials_2020.zip,* is a ZIP archive containing all of the presentations and sample Python files for all of the available Python tutorials.
    - This is for everyone, regardless of the specific Python tutorial you are taking.
    - This ZIP archive must be extracted to a folder to use it with the Python software.
      - Windows: right-click the ZIP file and choose “Extract All”
      - OSX: double-click the ZIP file
      - Linux: use the unzip utility from a terminal: `unzip rcs_py_tutorials_2020.zip`

SCC Python Tutorials

- Introduction to Python, Part one
- Introduction to Python, Part two
- Numerical and Scientific Computing in Python
- Python for Data Analysis
- Data Visualization in Python
- Introduction to Python Scikit-learn

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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: 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/

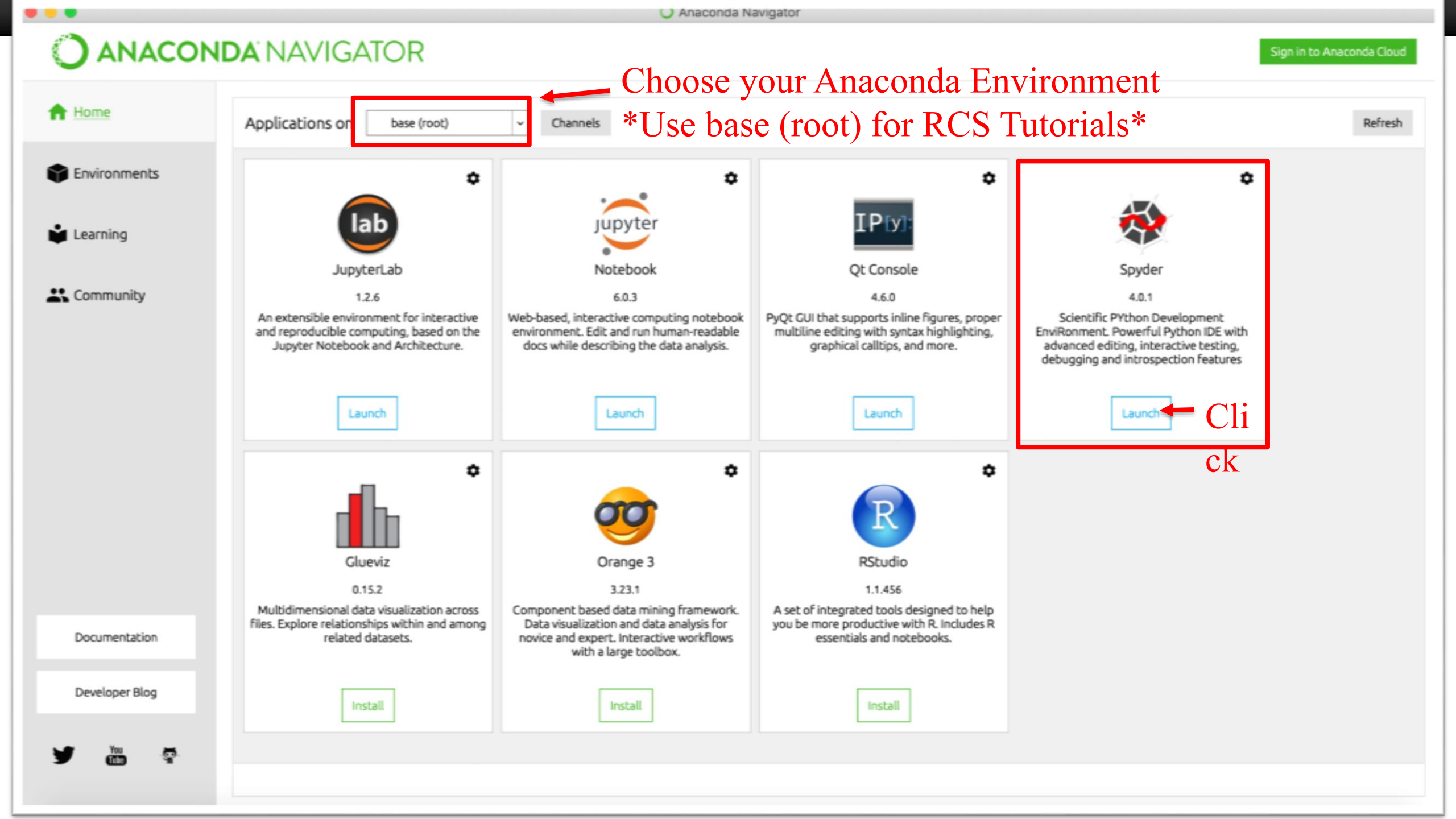
- Intel Python

BU's most popular personal 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.

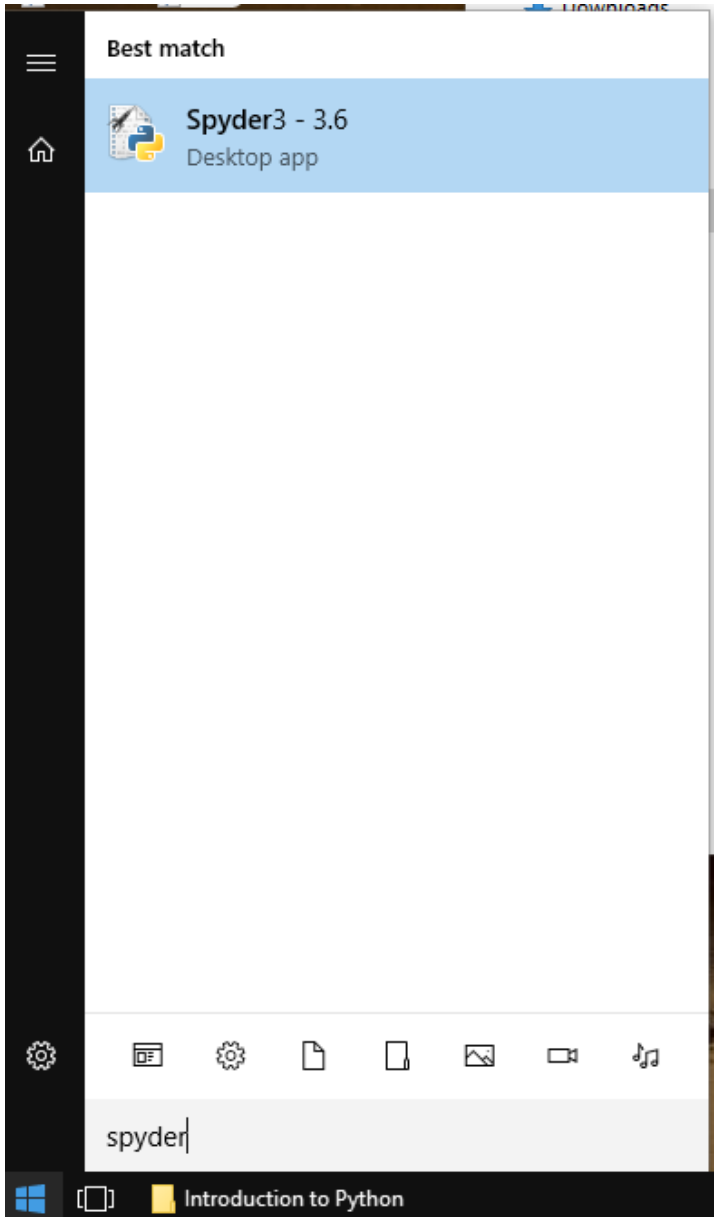
Python 2 vs. 3

- Python 2: released in 2000, Python 3 released in 2008
  - Python 2 is in “end-of-life” mode – no new releases or patches after Dec 31, 2019
  - No library support (e.g. pandas, numpy, etc.) after that date
  - For more: https://www.python.org/doc/sunset-python-2/
- Py3 is not completely compatible with Py2
  - For learning Python these differences are almost negligible
- Which one to learn?
  - **Python 3**
  - 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


Anaconda Navigator
ANACONDA NAVIGATOR
Sign in to Anaconda Cloud
Home
Environments
Learning
Community
Documentation
Developer Blog
Applications on
base (root)
Channels
Refresh
Choose your Anaconda Environment
Use base (root) for RCS Tutorials
JupyterLab
1.2.6
An extensible environment for interactive and reproducible computing, based on the Jupyter Notebook and Architecture.
Launch
Notebook
6.0.3
Web-based, interactive computing notebook environment. Edit and run human-readable docs while describing the data analysis.
Launch
Qt Console
4.6.0
PyQt GUI that supports inline figures, proper multiline editing with syntax highlighting, graphical calltips, and more.
Launch
Spyder
4.0.1
Scientific PYthon Development EnviRonment. Powerful Python IDE with advanced editing, interactive testing, debugging and introspection features
Launch
Click
Glueviz
0.15.2
Multidimensional data visualization across files. Explore relationships within and among related datasets.
Install
Orange 3
3.23.1
Component based data mining framework. Data visualization and data analysis for novice and expert. Interactive workflows with a large toolbox.
Install
RStudio
1.1.456
A set of integrated tools designed to help you be more productive with R. Includes R essentials and notebooks.
Install

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.
- Be patient…it takes a while to start.



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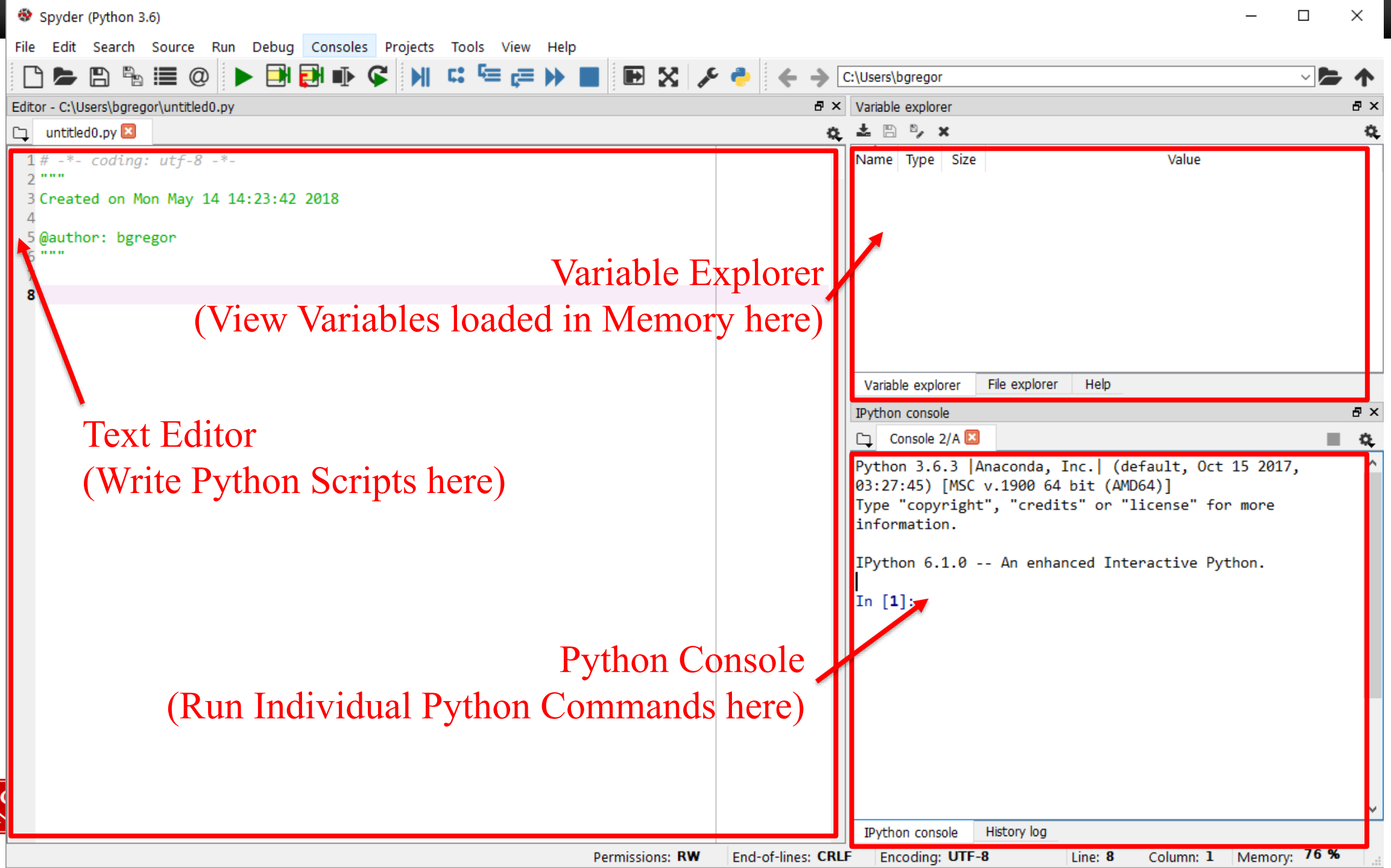
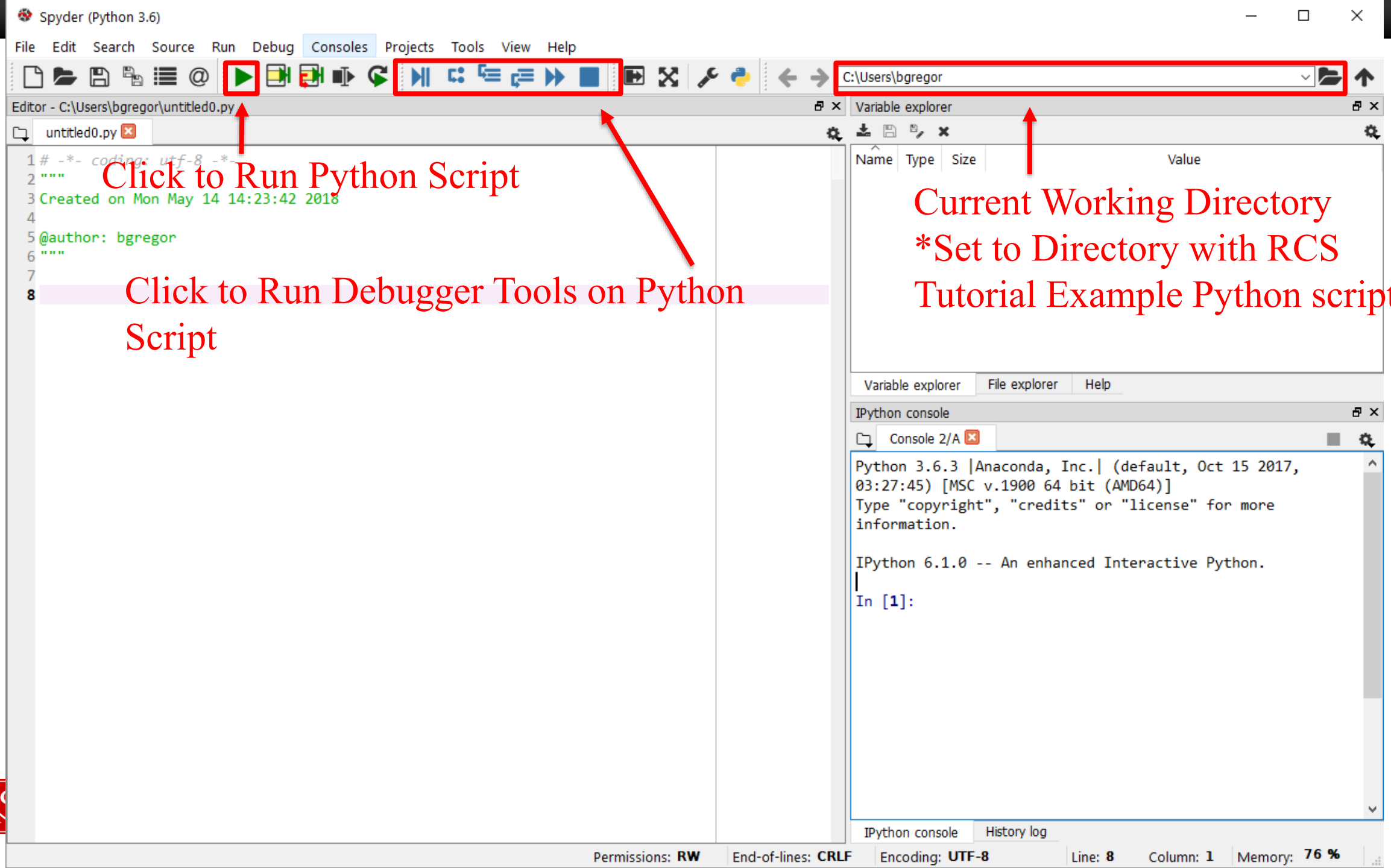
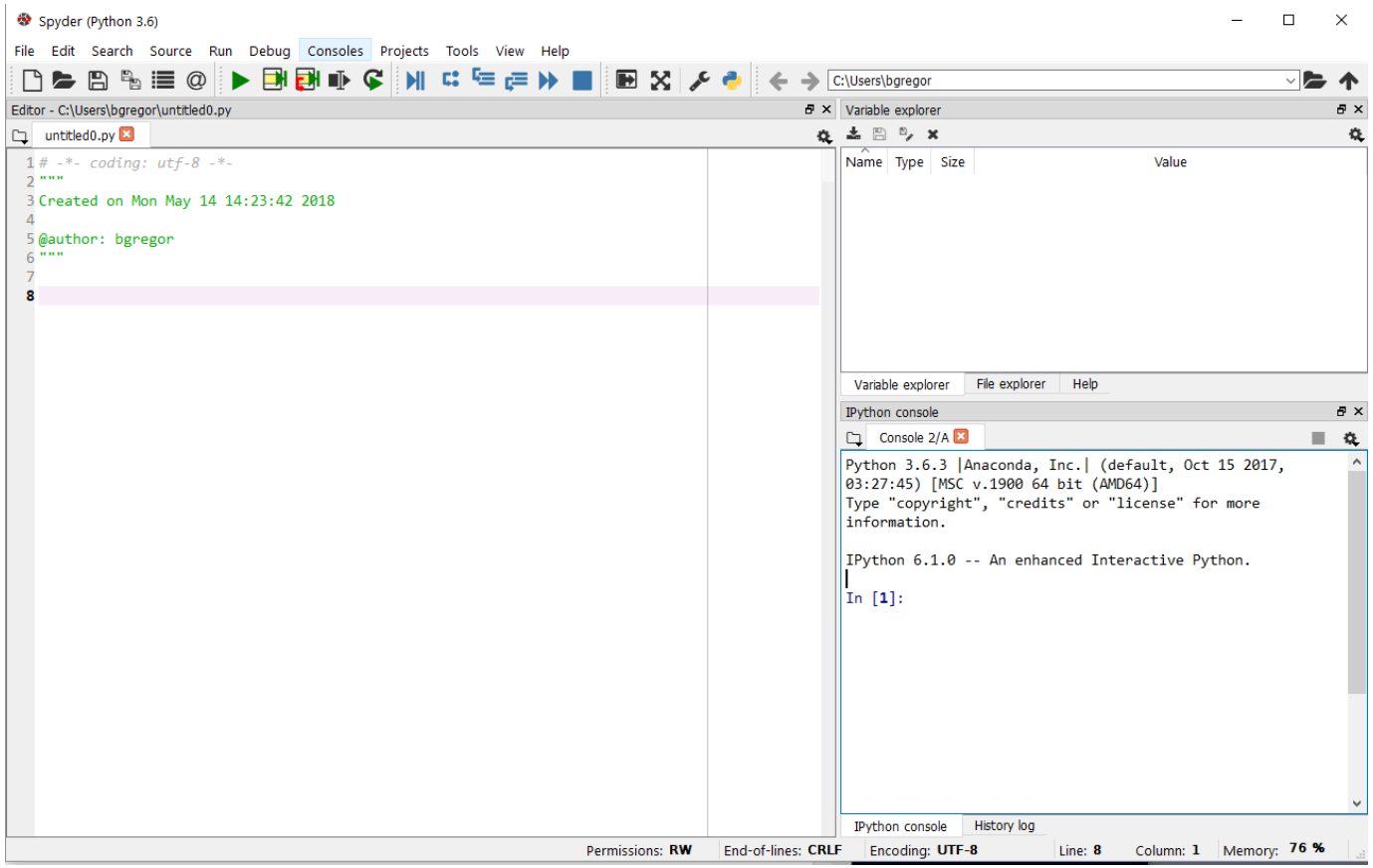

Spyder (Python 3.6)
File Edit Search Source Run Debug Consoles Projects Tools View Help
C:\Users\bgregor
Editor - C:\Users\bgregor\untitled0.py
untitled0.py
-*- coding: utf-8 -*-
"""
Created on Mon May 14 14:23:42 2018
@author: bgregor
"""
Variable explorer
Name Type Size Value
Variable explorer File explorer Help
IPython console
Console 2/A
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 console History log
Permissions: RW End-of-lines: CRLF Encoding: UTF-8 Line: 8 Column: 1 Memory: 76 %
Variable Explorer
(View Variables loaded in Memory here)
Text Editor
(Write Python Scripts here)
Python Console
(Run Individual Python Commands here)


Spyder (Python 3.6)
File Edit Search Source Run Debug Consoles Projects Tools View Help
C:\Users\bgregor
Editor - C:\Users\bgregor\untitled0.py
untitled0.py
1 # -*- coding: utf-8 -*-
2 """
3 Created on Mon May 14 14:23:42 2018
4
5 @author: bgregor
6 """
7
8
Click to Run Python Script
Click to Run Debugger Tools on Python Script
Variable explorer
Name Type Size Value
Current Working Directory
Set to Directory with RCS Tutorial Example Python scripts
Variable explorer File explorer Help
IPython console
Console 2/A
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 console History log
Permissions: RW End-of-lines: CRLF Encoding: UTF-8 Line: 8 Column: 1 Memory: 76 %

Spyder – a Python development environment

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

- Cons
  - Learning curve
  - Can add complexity to smaller problems



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Tutorial Outline – Part 1

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

Tutorial Outline – Part 2

- Lists
- Tuples and dictionaries
- Modules
- numpy and matplotlib modules
- Script setup
- Development notes

Tutorial Outline – Part 1

- What is Python?
- Operators
- Variables
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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.

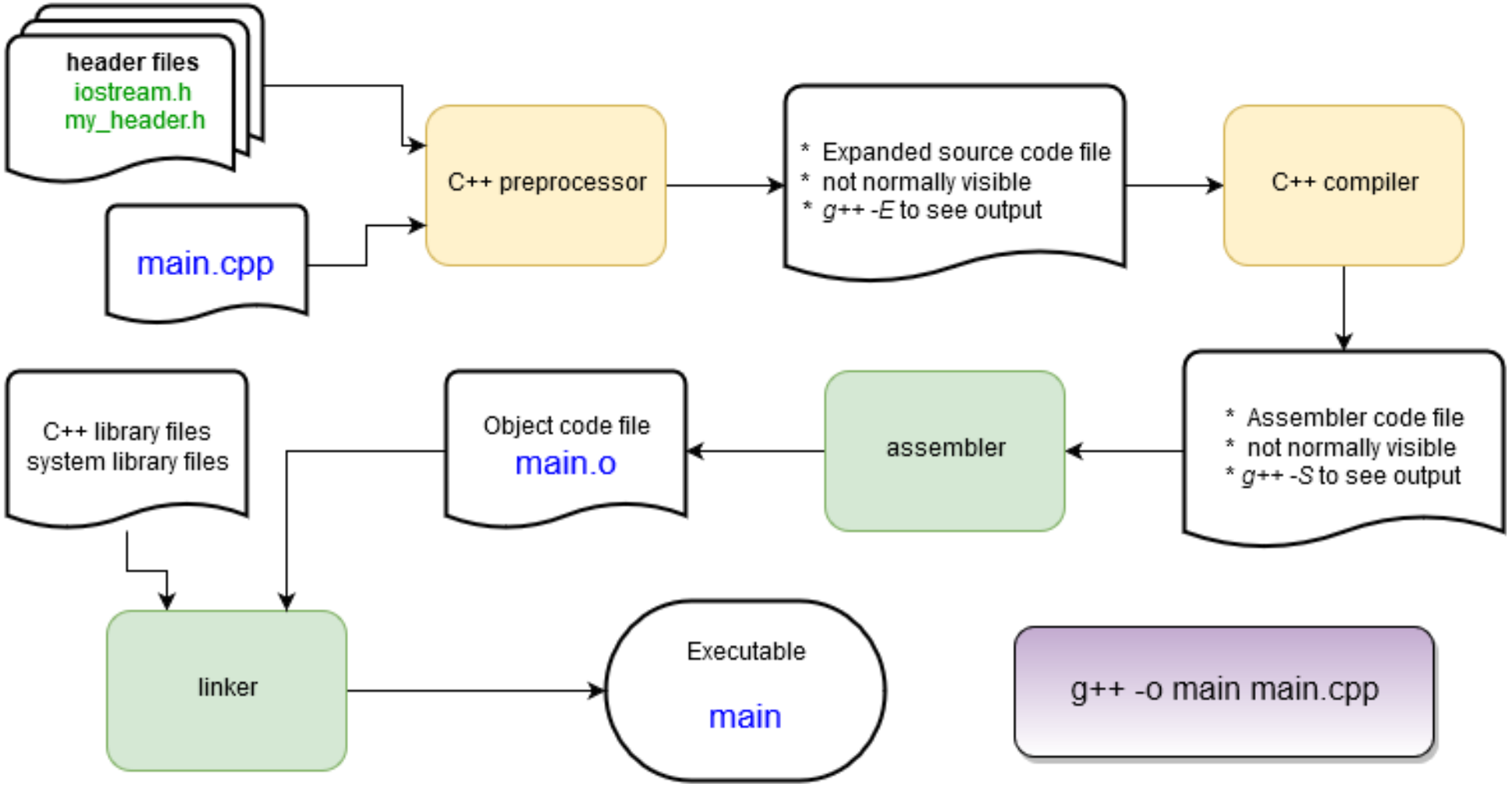
Some History

- “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).”

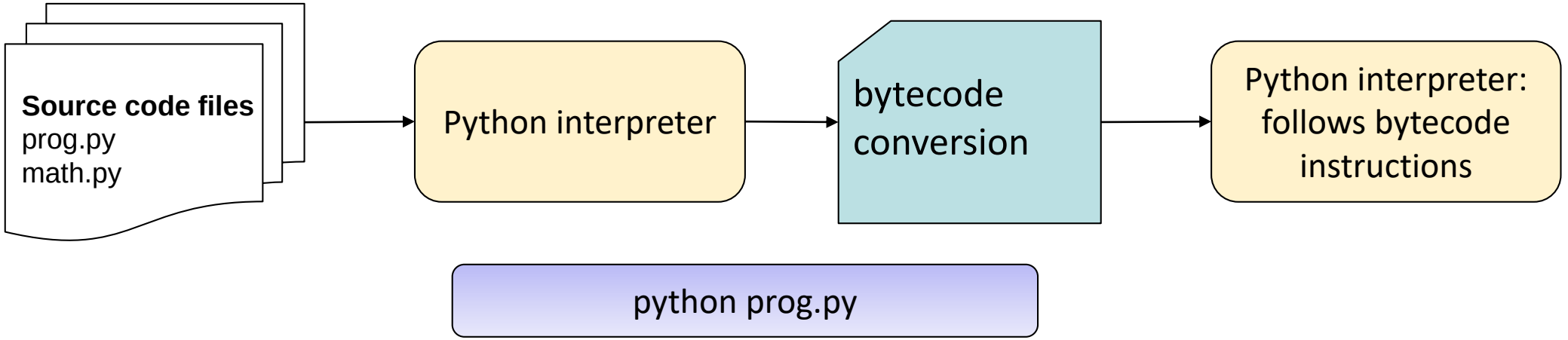
  –Python creator Guido Van Rossum, from the foreward to *Programming Python (1st ed.)*

- 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)



- A lot less work is done to get a program to start running compared with compiled languages!
- Python programs start running immediately – no waiting for the compiler to finish.
- 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
  - Compiler can optimize more extensively
- 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]:
```

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- IPython adds some handy behavior around the standard Python prompt.

Tutorial Outline – Part 1

- What is Python?
- Operators
- Variables
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Operators

- Python supports a wide variety of operators which act like functions, i.e. they do something and return a value:
  - Arithmetic: `+` `-` `*` `/` `%` `**`
  - Logical: `and` `or` `not`
  - Comparison: `>` `<` `>=` `<=` `!=` `==`
  - Assignment: `=`
  - Bitwise: `&` `|` `~` `^` `>>` `<<`
  - Identity: `is` `is not`
  - Membership: `in` `not in`

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?

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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]:
```

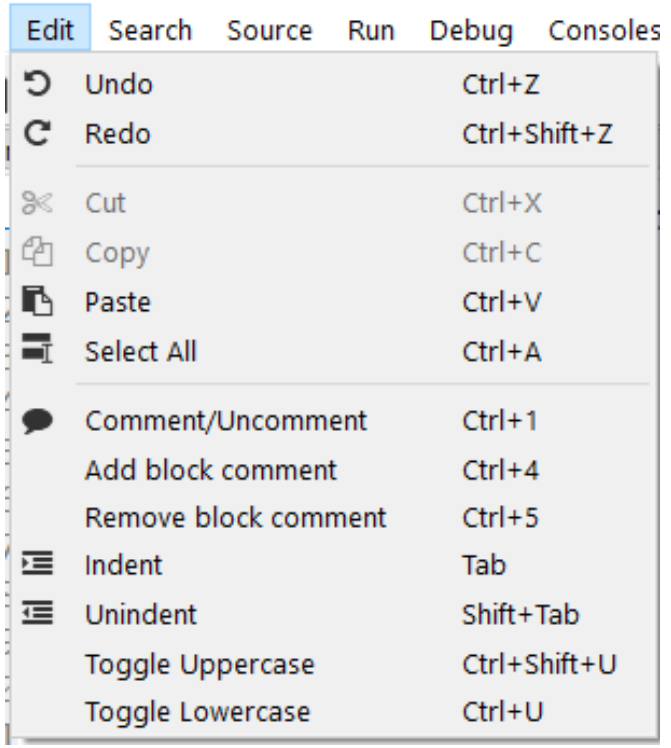
Comments

- # 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 vice-versa. Check the *Edit* menu

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



Tutorial Outline – Part 1

- What is Python?
- Operators
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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!**
  - Visualize Assignment

- 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
```

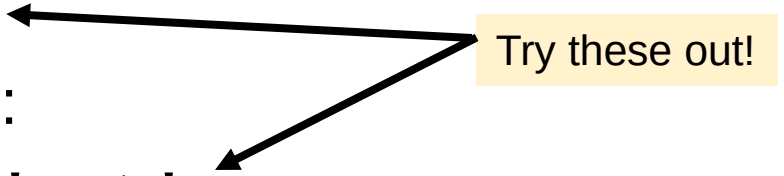
Variables cont'd

- Variables refer to a value stored in memory and are created when first assigned
- Variable names:
  - Must begin with a letter (a - z, A - Z) 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'
```



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**, **sets**, and **tuples**
    - These hold collections of variables
  - Specialty types: files, network connections, objects

- Custom types can be defined using Python classes.

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 *y* from *x*	x = x - y
x *= y	Multiply the value of *x* by *y*	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.

```
'cat'

"dog"

"What's that?"

'They said "hello"'

''' This is
    a multiline
    string '''
```

Tutorial Outline – Part 1

- What is Python?
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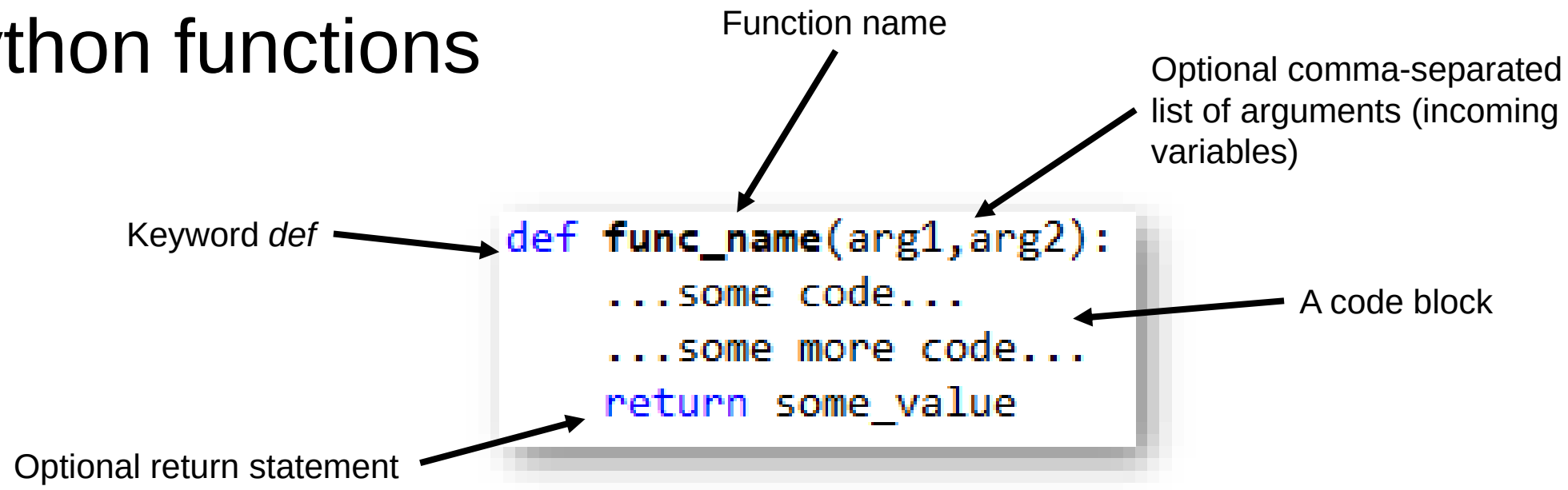
Functions

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

Python functions



- 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.

Which code sample is easier to read?

- C:

```c
float avg(int a, int b, int c){
float sum = a + b + c ;
return sum / 3.0 ;}
```

or

```c
float avg(int a, int b, int c)
{
   float sum = a + b + c ;
   return sum / 3.0 ;
}
```

- Matlab:

```matlab
function a = avg(x,y,z)
a = x + y + z ;
a = a / 3.0 ;
end
```

or

```matlab
function a = avg(x,y,z)
   a = x + y + z ;
   a = a / 3.0 ;
end
```

Which code sample is easier to read?

- Most languages use special characters ({ } pairs) or keywords (*end*, *endif*) to indicate sections of code that belong to:
  - Functions
  - Control statements like *if*
  - Loops like *for* or *while*
- Python instead uses the **indentation** that programmers use anyway for readability.

C

```c
float avg(int a, int b, int c)
{
    float sum = a + b + c ;
    return sum / 3.0 ;
}
```

Matlab

```matlab
function a = avg(x,y,z)
    a = x + y + z ;
    a = a / 3.0 ;
end
```

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 **:**

```
def avg(x,y,z):
        all_sum = x + y + z
        return all_sum / 3.0

def mean(x,y,z):
        return (x + y + z) / 3.0
```

A code block

Another code block

- This pattern is consistently repeated throughout Python syntax.
- Spaces or tabs can be mixed in a file but **not** within a code block.

Function Return Values

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

```
A = some_func()   # some_func returns 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
```

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Garbage collection

- Variables defined in a function no longer have any “live” references to them once the function returns.
- These variables become *garbage* – memory that can no longer be used.
- Python’s *garbage collection* operates to return that memory to the operating system so it can 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.

When does garbage collection occur?

- It happens when Python thinks it should.
  - Part of the process is based on heuristics, i.e. tuned parameters in Python.
  - For the **great** majority of programs this is not an issue.

- Programs that use plenty of small functions tend to create and reclaim intermediate variables or results and memory usage is better controlled.

- The takeaway: use functions, and plenty of them.

- If you are having trouble with memory usage contact RCS for help!

Tutorial Outline – Part 1

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

Classes

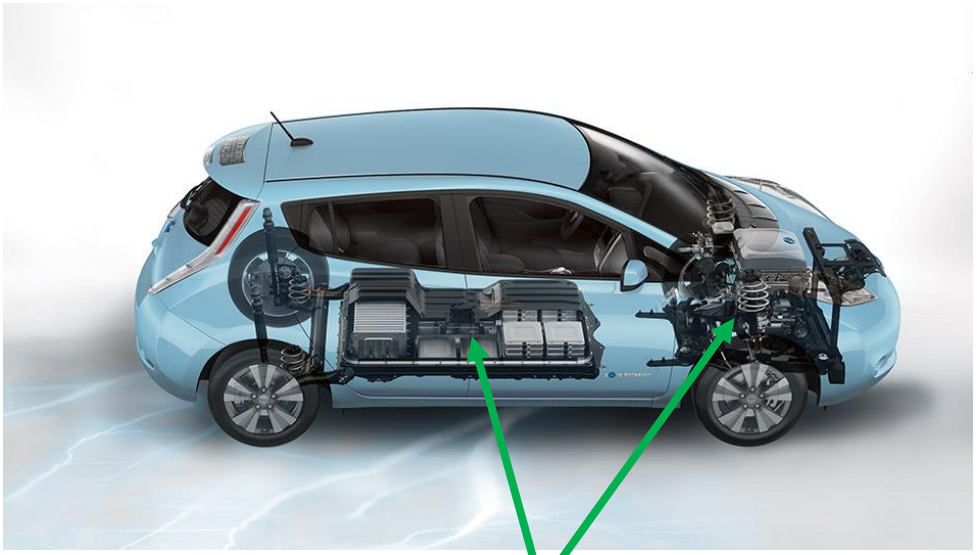
- OOP: Object Oriented Programming
- In OOP a *class* is a data structure that combines data with functions that operate on that data.
- An *object* is a variable whose type is a *class*
  - Also called an *instance* of a class
- Classes provide a lot of power to help organize a program and can improve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

Object-oriented programming

- Classes can contain data and methods (internal functions).
- Methods can call other code inside the class to implement complex behavior.
- This is a highly effective way of modeling real world problems inside of a computer program.

"Class Car"

public interface



internal data and methods

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Object-oriented programming

- Python is a fully object oriented programming (OOP) language.
- Some familiarity with OOP is needed to understand Python data structures and libraries.
- You can write your own Python classes to define custom data types.

Track via separate variables

```
boston_pop = 685094
boston_sq_km = 232.1
boston_num_colleges = 35
```

Boston	
Population	685094
Area (km^2)	232.1
# of colleges	35

A class lets you bundle these into one variable

Writing Your Own Classes

```
class Student:
    def __init__(self, name, buid, gpa):
        self.name = name
        self.buid = buid
        self.gpa = gpa

    def has_4_0(self):
        return self.gpa==4.0

me = Student("RCS Instructor","U0000000",2.9)
print(me.has_4_0())
```

- Your own classes can be as simple or as complex as you need.
- Define your own Python classes to:
  - Bundle together logically related pieces of data
  - Write functions that work on specific types of data
  - Improve code re-use
  - Organize your code to more closely resemble the problem it is solving.

Syntax for using Python classes

Create an object, which is a variable whose type is a Python class.

Created by a call to the class or returned from a function.

```
# Open a file. This returns a file object.
file = open('some_file.txt')

# Read a line from the text file.
line = file.readline()

# Get the filename
file.name # --> some_file.txt
```

Call a method for this object:

`object_name.method_name(args…)`

Access internal data for this object:

`object_name.data_name`

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Classes bundle data and functions

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

```
radius = 14.0
width_square = 14.0
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.

```
# create a Circle object with the radius value
c1 = Circle(radius)
r1 = Square(width_square)

a1 = c1.area()
a2 = r1.area()
```

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Strings in Python

- Python defines a string class – **all strings in Python are objects.**

- This means strings have:
  - Their own internal (hidden) memory management to handle storage of the characters.

  - A variety of methods (functions) accessible once you have a string object in memory.

- You can't access string functions without a string – in Python the string provides its own functions.
  - No "strcat" / "strcmp" / etc as in C
  - No "strlength" / "isletter" / etc as in Matlab
  - No "nchar" / "toupper" /etc as in R

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)

```
mystr = 'Hello!'

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 object that contains **any** countable thing.

```
len(mystr)→ 6
```

- 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.

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

- + concatenates strings.
- += appends strings.
  - These are defined in the string class as functions that operate on strings.

- 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' % variable
```

Variables are listed in the substitution order inside ()

- For more than one:

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

- Printing:

```
print('x: %s, y: %s, z:%s' % (xval,yval,2.0))
```

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String Substitutions (variations)

- There are 3 other ways to format strings…
- The “%s” approach is the original method.

- Alternative 1: f-strings

```
name = 'Boston'
f'{name} University'
```

- Alternative 2: string formatting

```
"{} University".format("Boston")
```

- Alternative 3: String templates. Part of the string library.

```
from string import Template
s = Template('$city $univ')
s.substitute(city='Boston',
             univ='University')
```

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When to use your own class

- A class works best when you've done some planning and design work before starting your program.
- This is a topic that is best tackled after you're comfortable with solving programming problems with Python.
- Some tutorials on using Python classes:

  W3Schools: https://www.w3schools.com/python/python_classes.asp

  Python tutorial: https://docs.python.org/3.6/tutorial/classes.html

Tutorial Outline – Part 1

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

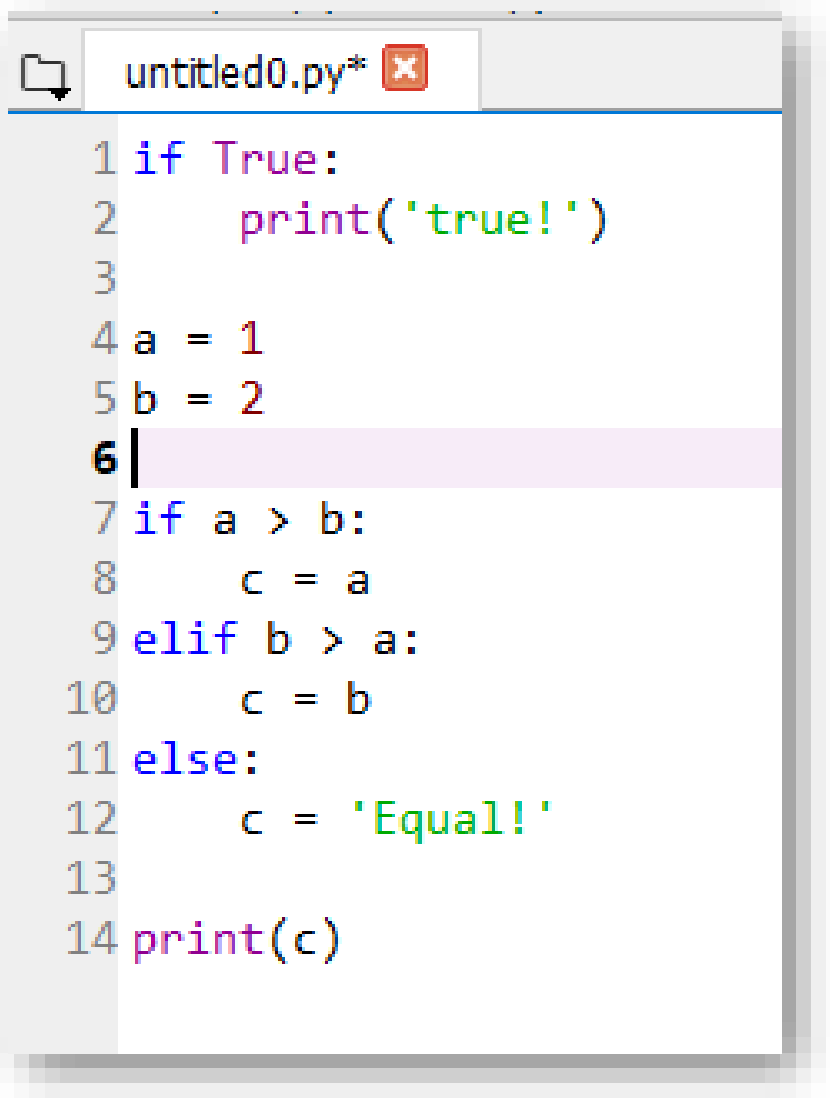
If / Else

- *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 – use them 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?



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')
```

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.
- This sometimes causes confusion when pasting code into the console.
  - Solution: try to avoid pasting more than a few lines into the Python console.