Introduction to Python
Part 1

v0.3

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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
  - ~17,000 CPUs running Linux

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

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About You

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

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Running Python for the Tutorial

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

```
module load anaconda3
spyder &
unzip /projectnb/scv/python/Intro_Python_code_0.3.zip
```

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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!

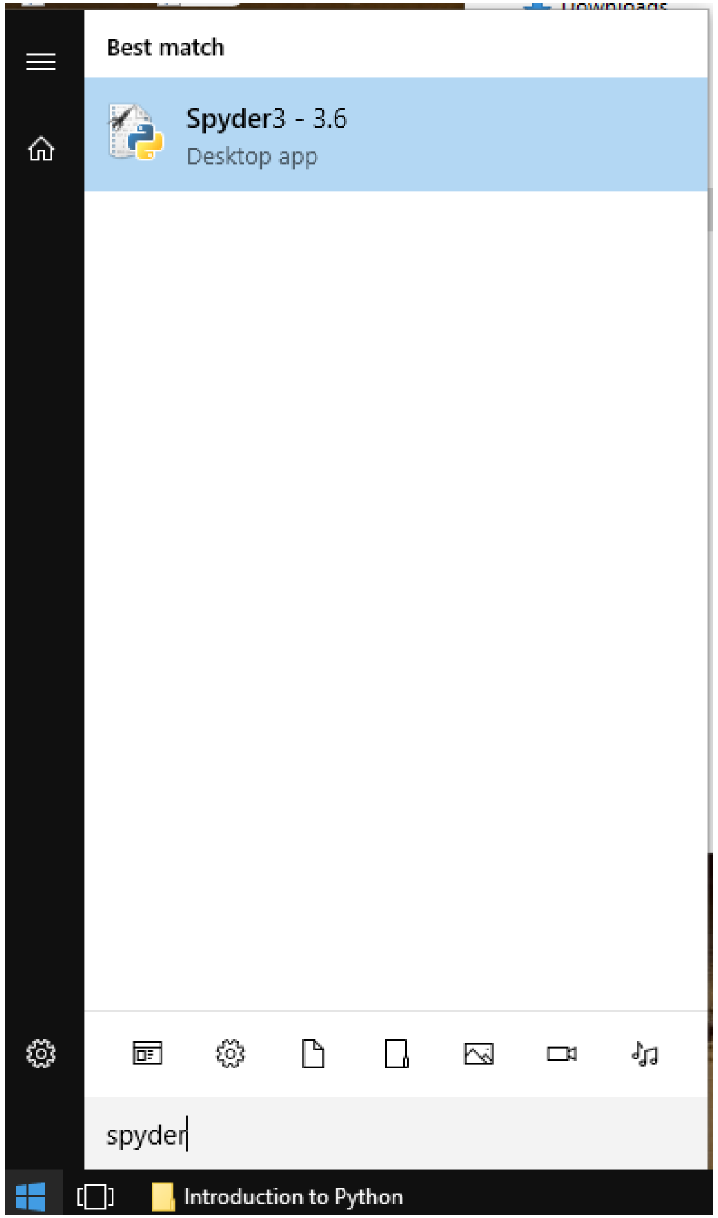
-

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.

- Be patient…it takes a while to start.



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.

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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!

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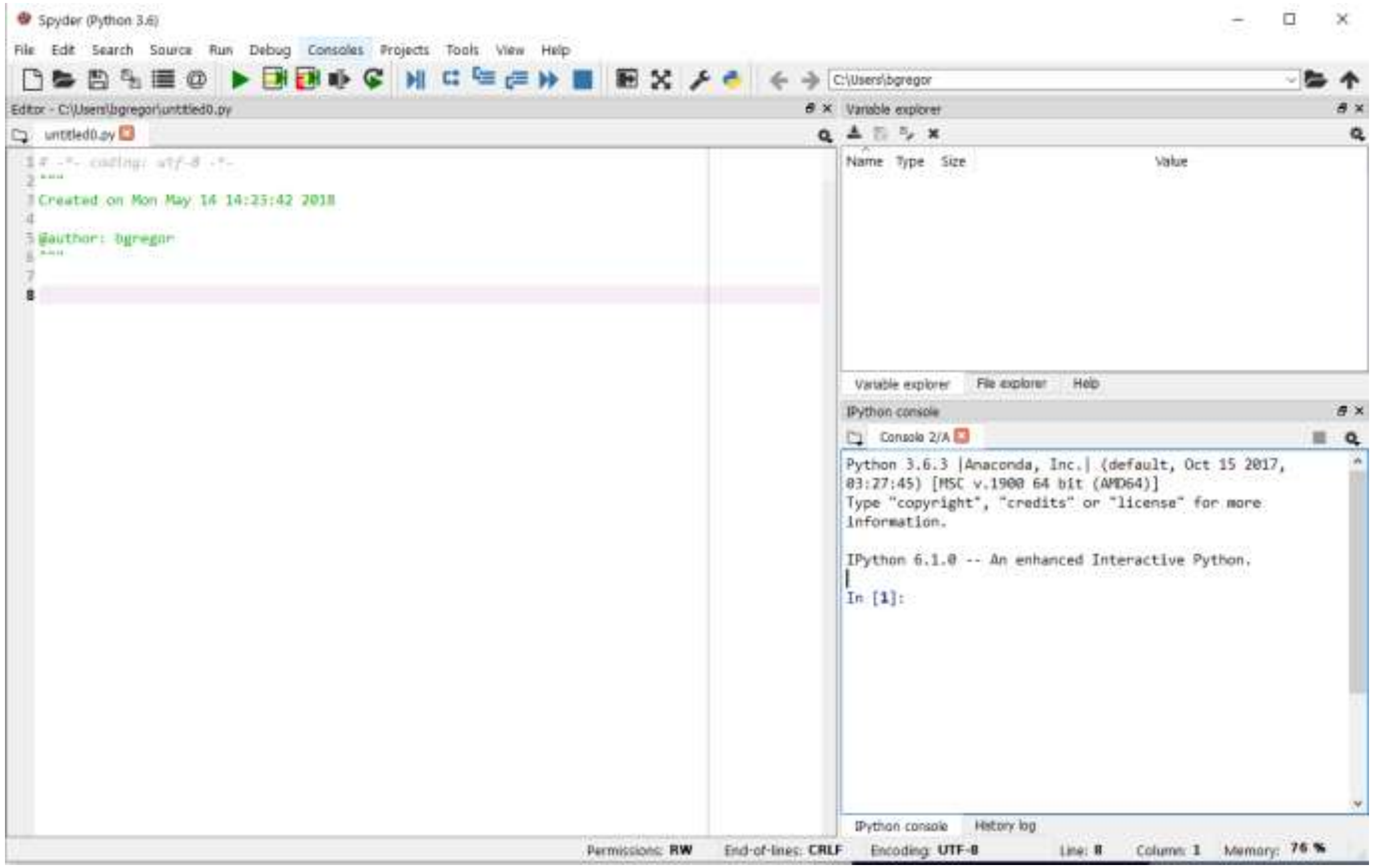
Spyder – a Python development environment

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

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



Tutorial Outline – Part 1

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

Tutorial Outline – Part 2

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

Tutorial Outline – Part 1

- What is Python?
- Operators
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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

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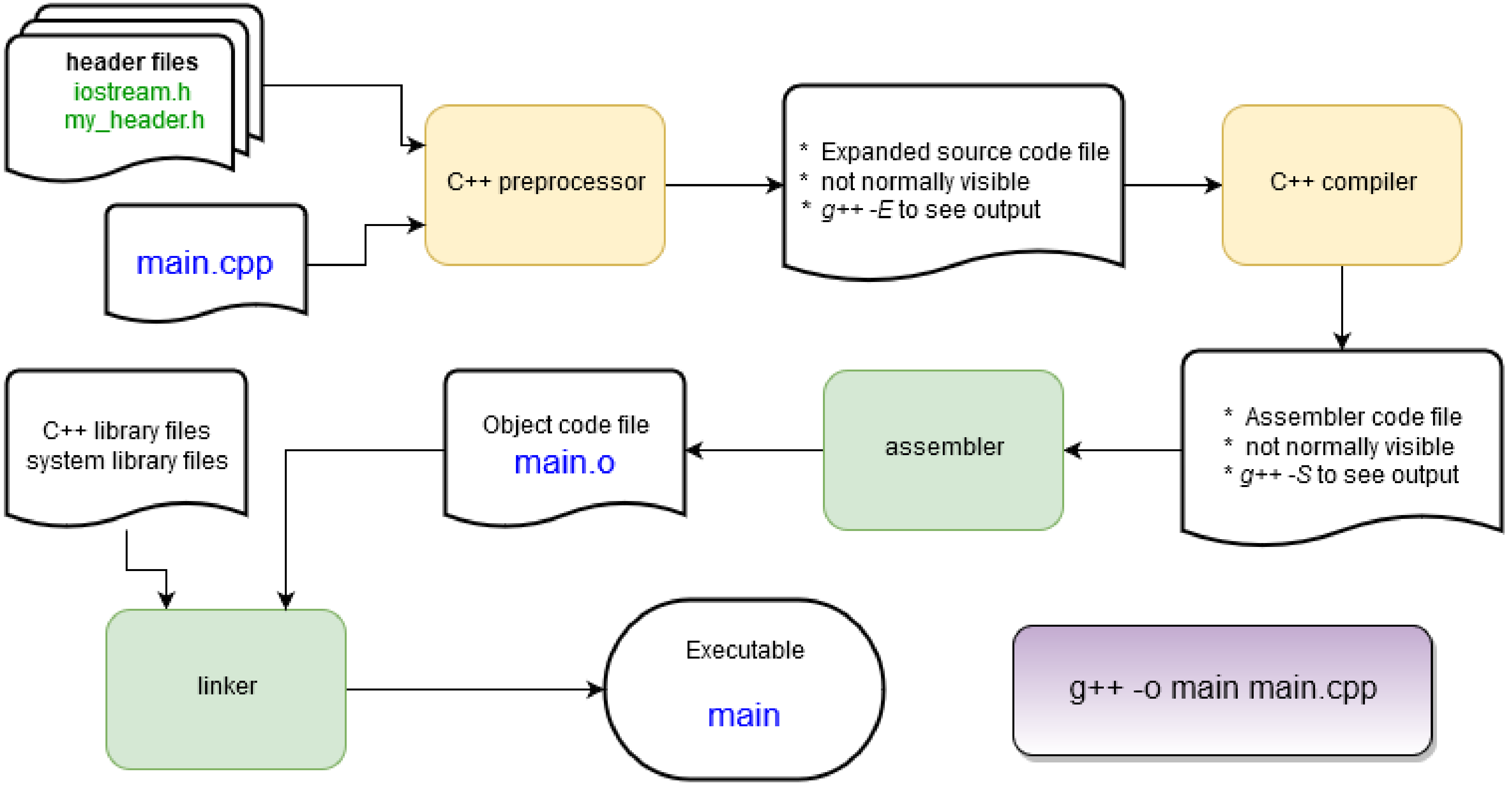
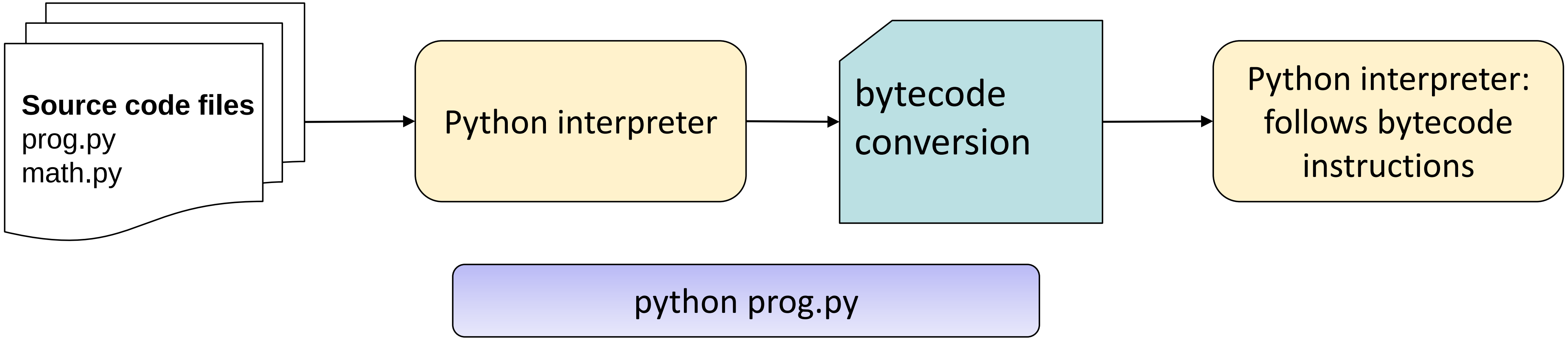
Compiled Languages (ex. C++ or Fortran)



Interpreted Languages (ex. Python or R)



- A lot less work is done to get a program to start running compared with compiled languages!
- 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

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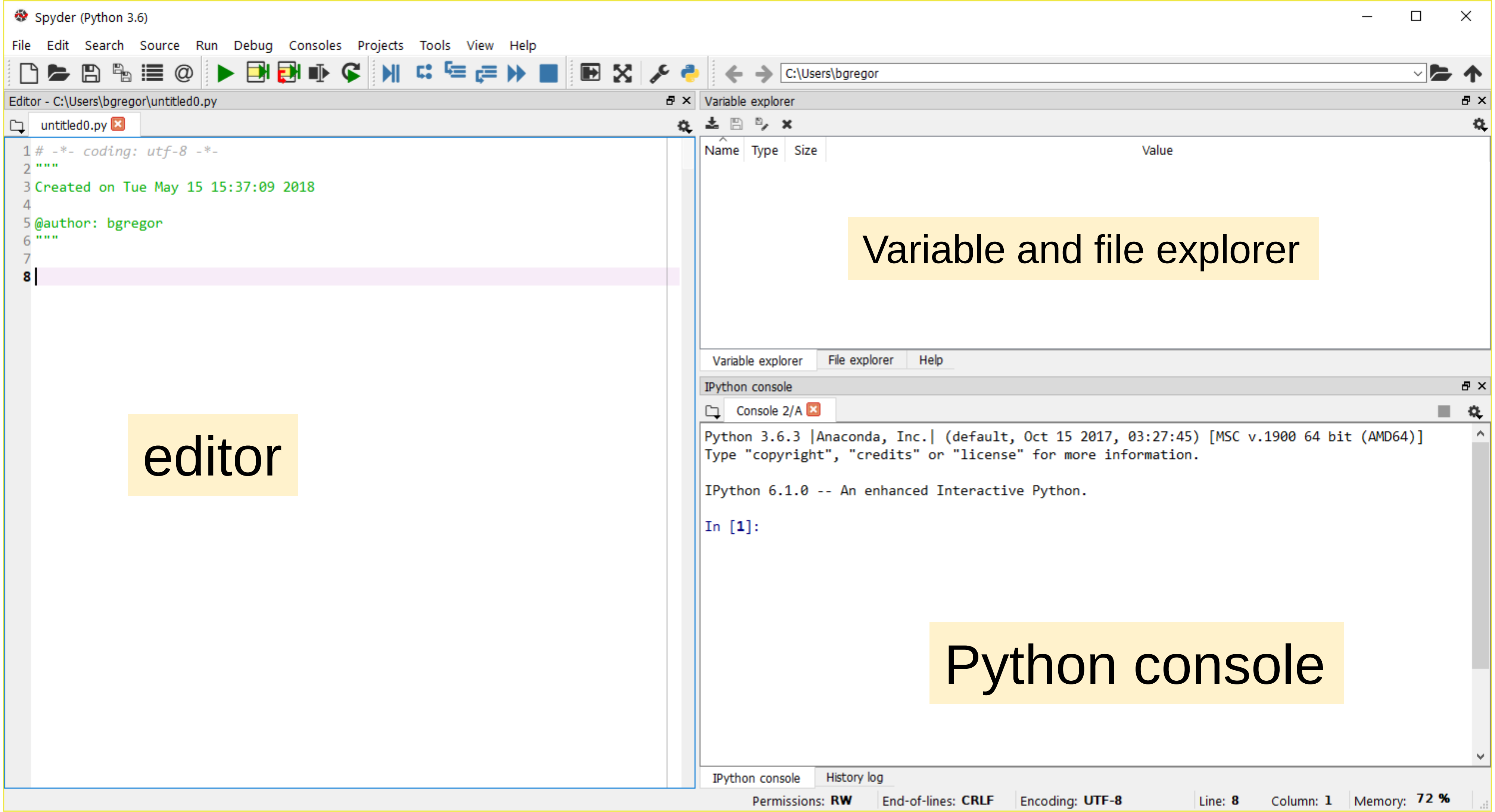
- IPython adds some handy behavior around the standard Python prompt.

The Spyder IDE



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- What is Python?
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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`

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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

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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]:
```

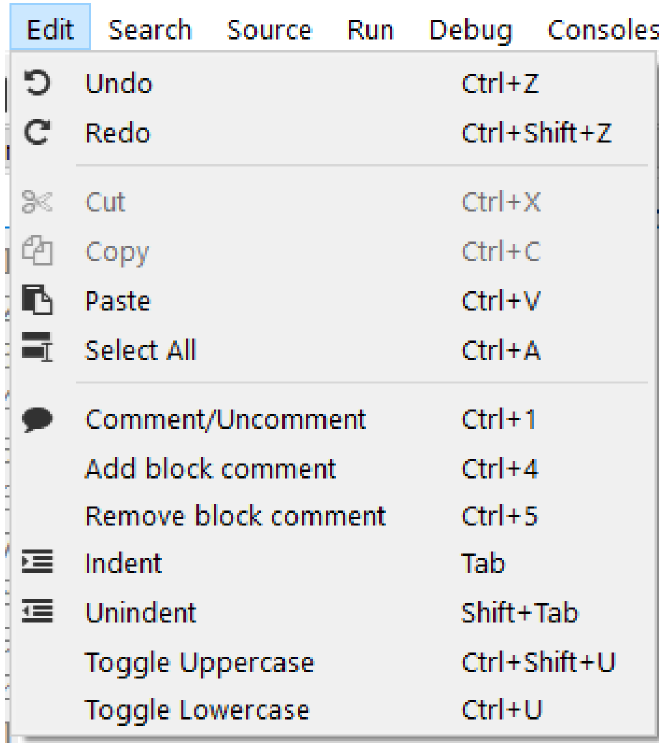
Comments

- # 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
```



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Tutorial Outline – Part 1

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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!

- 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!

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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!!

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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 *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!

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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 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.

Python functions

Function name

Optional comma-separated list of arguments (incoming variables)

Keyword *def*

```
def func_name(arg1,arg2):
    ...some code...
    ...some more code...
    return some_value
```

A code block

Optional return statement

- 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

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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?

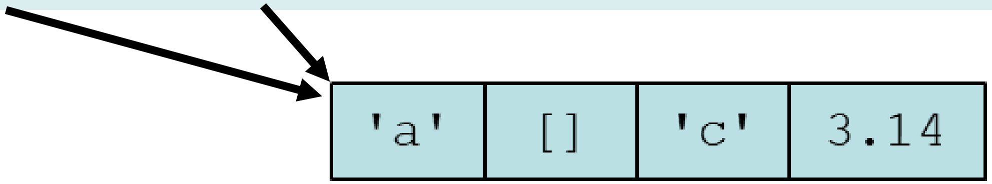
```
x = ['a', [], 'c', 3.14]
y=x  # y points to the same list as x
```

- 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!
```



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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?

- 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.

```python
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))
```

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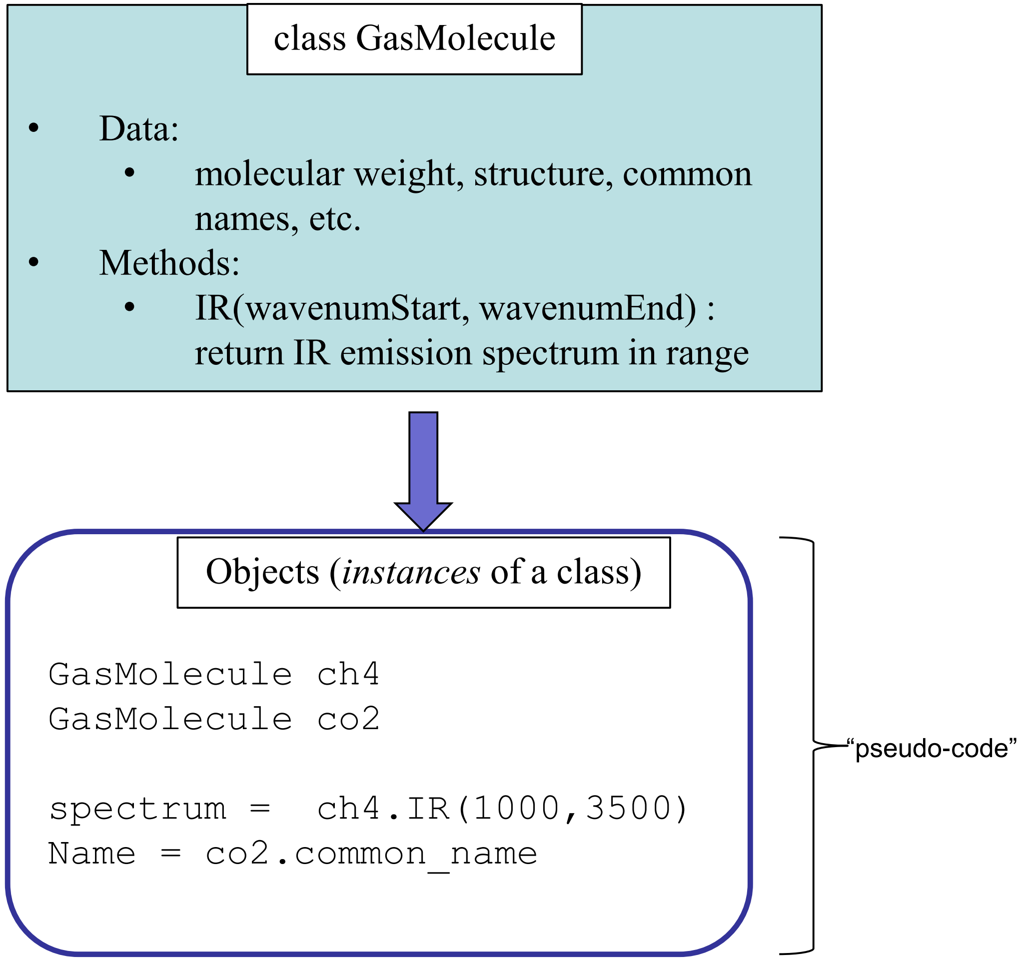
Classes

- 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.



Object-oriented programming

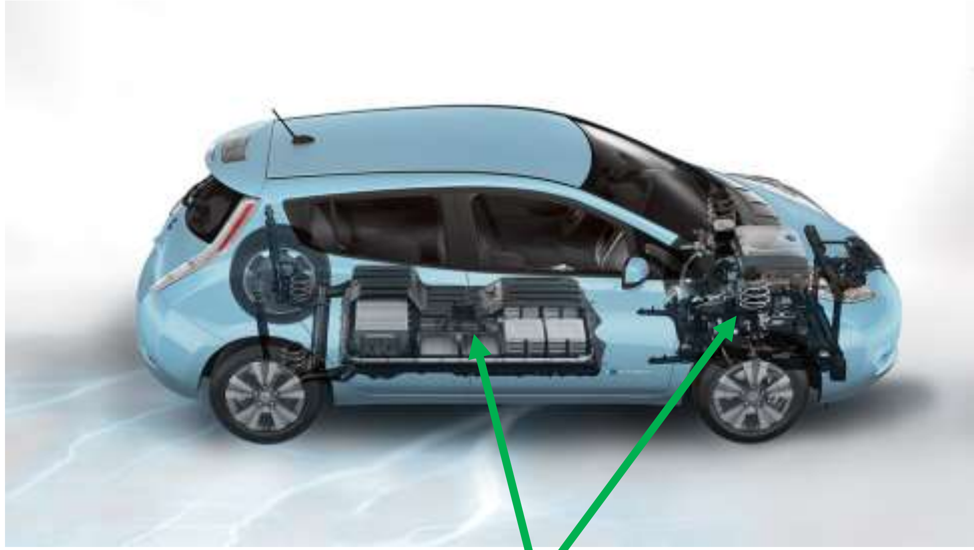
"Class Car"

- OOP defines *classes* to represent the parts of the program.
- Classes can contain data and methods (internal functions).

- 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



private data and methods

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Encapsulation bundles data and functions

- 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 (hidden) memory management to handle storage of the characters.
  - A variety of functions accessible once you have a string object in memory.

- You can’t access string functions without a string!
  - No “strcat” / “strcmp” / … as in C
  - No “strlength” / “isletter” / … as in Matlab

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 object that contains **any** 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.

```
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] = 'O'
Traceback (most recent call last):

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

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

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

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String Substitutions

%s means sub in value

variable name comes after a %

- Python provides an easy way to stick variable values into strings called *substitutions*

- Syntax for one variable:

```
'string with a %s' % variable
```

- For more than one:

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

Variables are listed in the substitution order inside ()

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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*

```python
if True:
    print('true!')

a = 1
b = 2

if a > b:
    c = a
elif b > a:
    c = b
else:
    c = 'Equal!'

print(c)
```

Indentation of code…easier on the eyes!

- C:

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

or

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

- Matlab:

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

or

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

```
if 3 > 4:
    x = 5
else:
    x = 6
```

A code block (x = 5)

Another code block (x = 6)

- 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')
```

- Note the lack of “end if”, “end”, curly braces, etc.

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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.

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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**!

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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

```
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]
```

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

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']
```

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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]`

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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]` → `'a'`
- Nth element: `x[2]` → `'c'`
- Last element: `x[-1]` → `'e'`
- Next-to-last: `x[-2]` → `'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**

- `x[0:1]` → `['a']`
- `x[0:2]` → `['a','b']`
- `x[-3:]` → `['c', 'd', 'e']   # Third from the end to the end`
- `x[2:5:2]` → `['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` → x is now `[-3.14, 'b', 'c', 'd', 'e']`
- `del x[-1]` → 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

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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]

y = 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('y: %s' % y)
```

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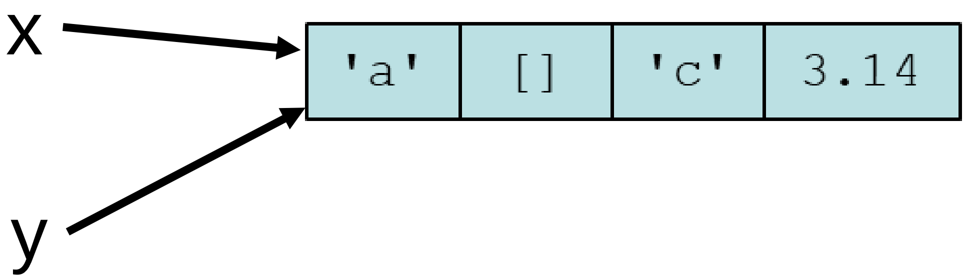
Variables and Memory Locations

- 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.
- This is how all objects in Python are handled.

```
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.

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 1st 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):
    print( my_list[i] )
    i += 1
    if i==3:
        break
```

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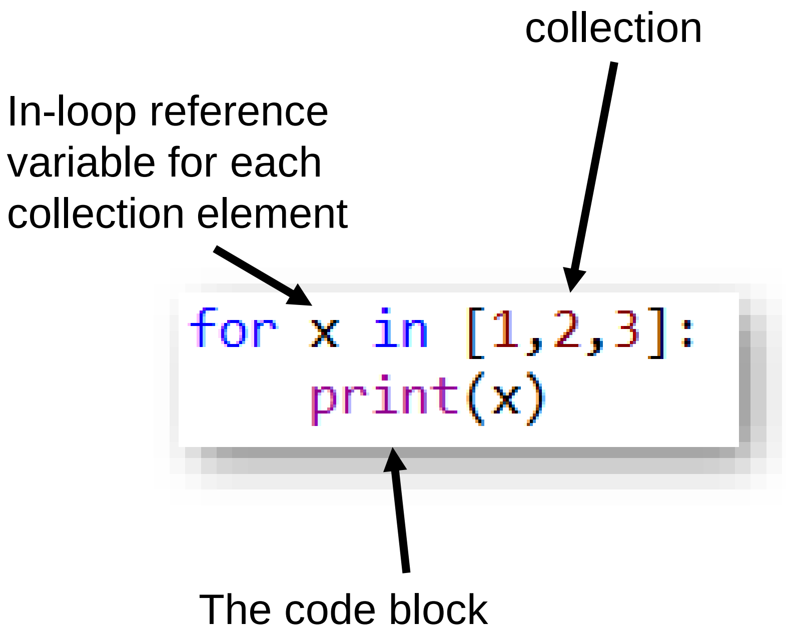
For loops

- *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.

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The range() function

- The range() function auto-generates sequences of numbers that can be used for indexing into lists.

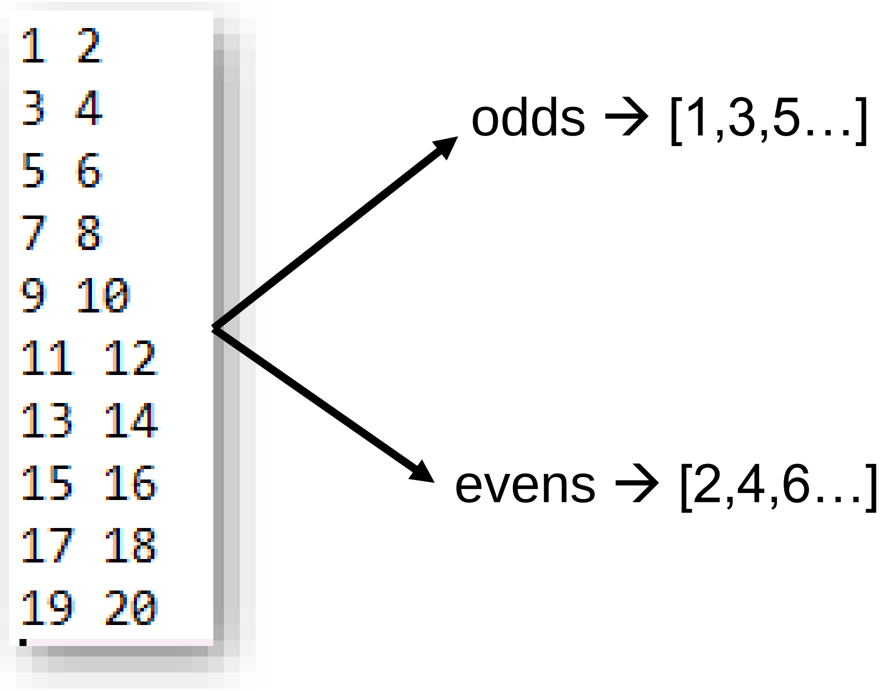
- Syntax: range(*start*, *exclusive end*, *increment)*

- range(0,4) → produces the sequence of numbers 0,1,2,3
- range(-3,15,3) → -3,0,3,6,9,12
- range(4,-3,2) → 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!

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