

Computational Materials Python Cheat Sheet

This cheat sheet was created in python's interactive mode. In the interactive mode you type commands into the interpreter and directly find out the results. The ">>>" is the prompt used to let you know that python is ready to accept a command. To start python in interactive mode type **python** on command line. It will look as follows:

```
[wc5879@fri ~]$ python
Python 2.7.1 (r271:86832, May 29 2012, 13:10:45)
[GCC 4.4.6 20110731 (Red Hat 4.4.6-3)] on linux2
Type "help", "copyright", "credits" or "license" for more information.
>>> █
```

Below are examples of how to use the python programming language.

Variable Assignments

>>> x=5 >>>x 5	Declaring an integer variable x with value 5 or assign variable x to the integer 5
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Types of Variables

>>> name = 'Bob' >>> I=5 >>> F=5.0 >>> happy='True'	String Integer Float Bool
--	------------------------------------

Calculations with variables or arithmetic operators

>>>y=7 >>>y+5 12 >>>y-5 2 >>>y*2 14 >>>y**2 49 >>>y%2 1 >>>y/14 0 >>>y/14.0 0.5	Sum of two variables Subtraction of two variables Multiplication of two variables Exponential of two variables Remainder of a variable Division of two integers Division with at least one float
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Type Conversion or Type Casting

>>>str('5.1') 5.1 >>>int(5.0) 5 >>>float(5) 5.0 >>> type(5.4) <type 'float'>	Variables to strings Variables to integers Variables to float Returns variable type
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Lists

```
>>>Names = ['bob', 'finn', 'ray']
>>>Names
['bob', 'finn', 'ray']
>>>Names[0]
'bob'
>>>Names[-1]
'ray'
>>>Names[2]
'ray'
>>>len(list)
3
```

Note python starts its indexing/numbering at 0 not 1
Select item at index 0
Select last item in the list
Select third item in list
Returns length of list

Boolean Operators

```
>>> x=5
>>> x==5
True
>>> x!=5
False
>>> x>5
False
>>> x<=5
True
>>> True and True
True
>>> True and False
False
>>> True or True
True
>>> True or False
True
```

Equality: are the two values equal?
Inequality: are the two values not equal?
Greater than
Less than or equal to
Are both values True?
Are either values True?

If Statements (Recall indentation rules in python!)

```
>>> x=5
>>> if x==5:
...     print True
...
True
>>> if x==5:
...     print True
... else:
...     print False
...
True
>>> if x==2:
...     print 'value = 2'
... elif x<2:
...     print 'value < 2'
... else:
...     print 'value > 2'
...
value > 2
```

If conditional statement is True
then do

If conditional statement is True
then do
otherwise
do

If the conditional statement is True
do this
else if this conditional statement is True
do this
otherwise
do this

Loops

```
>>> x=0  
>>> while x < 5:  
...     print x  
...     x += 1  
  
...  
0  
1  
2  
3  
4
```

While the variable x is less than 5,
Print the value of x
And add one to the value of x

Output from while loop

```
>>> for i in range(0,5):  
...     print i  
...  
0  
1  
2  
3  
4  
>>>
```

For i ranging from 0 until 5
Print the value of i

Output from for loop

Defining functions

```
>>> def print_number(x):  
...     print x  
...  
>>> print_number(4)  
4  
  
>>> def return_number_add_one(x):  
...     return x+1  
...  
>>>  
new_number=return_number_add_one(5)  
>>> print new_number  
6  
>>>
```

Define the function which prints
the input value, x.

Call the function with input
value x=4.

Define a function which *returns*
the input value, x, plus one

Call the function and set the
output equal to new_number

Importing modules – Numpy

```
>>> import numpy  
>>> numpyarray =  
numpy.array([1,2,3],float)  
>>> numpyarray  
array([ 1.,  2.,  3.])  
>>> numpy.mean(numpyarray)  
2.0
```

Import module (numpy)
Create a numpy array of floats called
numpyarray

Use numpy to calculate the mean of the
values in numpyarray

If you want to find more numpy functions, try googling numpy + (insert
function your need!).