

January 27-29, 2015 PRACE Advanced Training Centre CSC – IT Center for Science Ltd, Finland

```
import sys, os
try:
    from Bio.PDB import PDBParser
     biopython_installed_ = True
except ImportError:
    __biopython_installed__ = False
  default_bfactor__ = 0.0  # default B-factor
 _default_occupancy__ = 1.0  # default occupancy level
_default_segid__ = ''  # empty segment ID
class EOF(Exception):
    def __init__(self): pass
class FileCrawler:
    Crawl through a file reading back and forth without loading
    anything to memory.
    def __init__(self, filename):
            self.__fp__ = open(filename)
        except IOError:
            raise ValueError, "Couldn't open file '%s' for reading." % filename
        self.tell = self.__fp__.tell
        self.seek = self.__fp__.seek
    def prevline(self):
        try:
             self.prev()
```



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Agenda

Tuesday

9:00-9:45	Introduction to Python
9:45-10:30	Exercises
10:30-10:45	Coffee Break
10:45-11:15	Control structures
11:15-12:15	Exercises
12:15-13:00	Lunch break
13:00-13:30	Functions and modules
13:30-14:30	Exercises
14:30-14:45	Coffee Break
14:45-15:15	File I/O and text processing
15:15-16:15	Exercises

Wednesday

9.00-9.45	Object oriented programming with Python
9.45-10.30	Exercises
10.30-10.45	Coffee break
10:45-11:15	NumPy – fast array interface to Python
11:15-12:15	Exercises
12.15-13.00	Lunch break
13.00-13:30	NumPy (continued)
13:30-14:30	Exercises
14.30-14.45	Coffee break
14.45-15.15	NumPy (continued)
15:15-16:15	Exercises

Thursday

9:00-9:45	Visualization with Python
9:45-10:30	Exercises
10:30-10:45	Coffee Break
10:45-11:30	Scipy-package for scientific computing
11:30-12:15	Exercises
12:15-13:00	Lunch break
13:00-13:30	C extensions – integrating efficient C routines in Python
13:30-14:30	Exercises
14:30-14:45	Coffee break
14:45-15:45	MPI and Python – mpi4py
15:45-16:15	Exercises



What is Python?

- Modern, interpreted, object-oriented, full featured high level programming language
- Portable (Unix/Linux, Mac OS X, Windows)
- Open source, intellectual property rights held by the Python Software Foundation
- Python versions: 2.x and 3.x
 - 3.x is not backwards compatible with 2.x
 - This course uses 2.x version

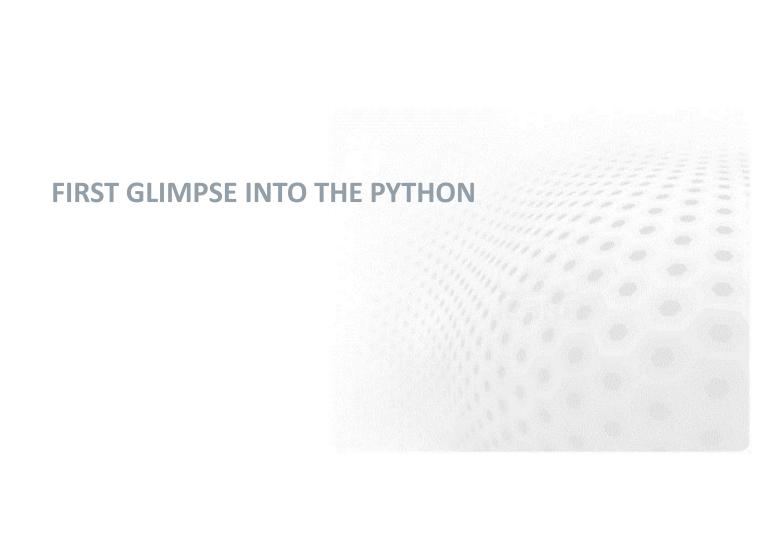
Why Python?

- Fast program development
- Simple syntax
- Easy to write well readable code
- Large standard library
- Lots of third party libraries
 - Numpy, Scipy, Biopython
 - Matplotlib

— ...

Information about Python

- www.python.org
- H. P. Langtangen, "Python Scripting for Computational Science", Springer
- www.scipy.org
- matplotlib.sourceforge.net
- mpi4py.scipy.org



Python basics

- Syntax and code structure
- Data types and data structures
- Control structures
- Functions and modules
- Text processing and IO

Python program

Typically, a .py ending is used for Python scripts, e.g. hello.py:

```
hello.py
print "Hello world!"
```

Scripts can be executed by the python executable:

```
$ python hello.py
Hello world!
```

Interactive python interpreter

The interactive interpreter can be started by executing python without arguments:

```
$ python
Python 2.4.3 (#1, Jul 16 2009, 06:20:46)
[GCC 4.1.2 20080704 (Red Hat 4.1.2-44)] on linux2
Type "help", "copyright", "credits" or "license" for more information.
>>> print "Hello"
Hello
>>>
```

Useful for testing and learning

Python syntax

- Variable and function names start with a letter and can contain also numbers and underscores, e.g "my_var", "my_var2"
- Python is case sensitive
- Code blocks are defined by indentation
- Comments start by # sign

```
example.py
# example
if x > 0:
    x = x + 1 # increase x
    print("increasing x")
else:
    x = x - 1
    print "decreasing x"
print("x is processed")
```

Data types

- Python is dynamically typed language
 - no type declarations for variables
- Variable does have a type
 - incompatible types cannot be combined

```
print "Starting example"
x = 1.0
for i in range(10):
    x += 1
y = 4 * x
s = "Result"
z = s + y # Error
```

Numeric types

- Integers
- Floats
- Complex numbers
- Basic operations
 - + and -
 - * , / and **
 - implicit type conversions
 - be careful with integer division!

```
>>> x = 2
>>> x = 3.0
>>> x = 4.0 + 5.0j
>>>
>>> 2.0 + 5 - 3
4.0
>>> 4.0**2 / 2.0 * (1.0 - 3j)
(8-24j)
>>> 1/2
0
>>> 1./2
0.5
```

Strings

- Strings are enclosed by " or '
- Multiline strings can be defined with three double quotes

```
strings.py
s1 = "very simple string"
s2 = 'same simple string'
s3 = "this isn't so simple string"
s4 = 'is this "complex" string?'
s5 = """This is a long string
expanding to multiple lines,
so it is enclosed by three "'s.""
```

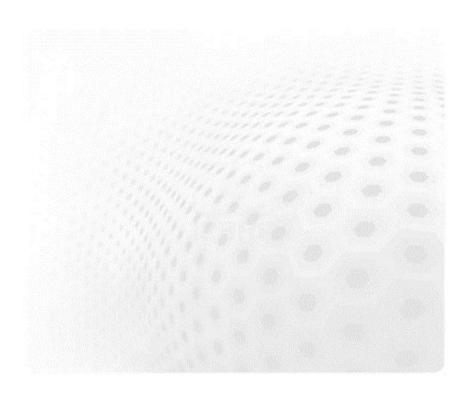
Strings

+ and * operators with strings:

```
>>> "Strings can be " + "combined"
'Strings can be combined'
>>>
>>> "Repeat! " * 3
'Repeat! Repeat! Repeat!
```

Data structures

- Lists and tuples
- Dictionaries



List

- Python lists are dynamic arrays
- List items are indexed (index starts from 0)
- List item can be any Python object, items can be of different type
- New items can be added to any place in the list
- Items can be removed from any place of the list

Lists

- Defining lists
- Accessing list elements

Modifying list items

```
>>> my_list1 = [3, "egg", 6.2, 7]
>>> my_list2 = [12, [4, 5], 13, 1]
```

```
>>> my_list1[0]
3
>>> my_list2[1]
[4, 5]
>>> my_list1[-1]
7
```

```
>>> my_list1[-2] = 4
>>> my_list1
[3, 'egg', 4, 7]
```

Lists

- Adding items to list
- Accessing list elements

+ and * operators with lists

```
>>> my_list1 = [9, 8, 7, 6]
>>> my_list1.append(11)
>>> my_list1
[9, 8, 7, 6, 11]
>>> my_list1.insert(1,16)
>>> my_list1
[9, 16, 8, 7, 6, 11]
>>> my_list2 = [5, 4]
>>> my_list1.extend(my_list2)
>>> my_list1
[9, 16, 8, 7, 6, 11, 5, 4]
```

```
>>> [1, 2, 3] + [4, 5, 6]
[1, 2, 3, 4, 5, 6]
>>> [1, 2, 3] * 2
[1, 2, 3, 1, 2, 3]
```

Lists

It is possible to access slices of lists

Removing list items

```
>>> my_list1 = [0, 1, 2, 3, 4, 5]
>>> my_list1[0:2]
[0, 1]
>>> my_list1[:2]
[0, 1]
>>> my_list1[3:]
[3, 4, 5]
>>> my_list1[0:6:2]
[0, 2, 4]
>>> my_list1[::-1]
[5, 4, 3, 2, 1, 0]
```

```
>>> second = my_list1.pop(2)
>>> my_list1
[0, 1, 3, 4, 5]
>>> second
2
```

Tuples

- Tuples are immutable lists
- Tuples are indexed and sliced like lists, but cannot be modified

```
>>> t1 = (1, 2, 3)
>>> t1[1] = 4
Traceback (most recent call last):
   File "<stdin>", line 1, in
<module>
TypeError: 'tuple' object does not
support item assignment
```

Dictionaries

- Dictionaries are associative arrays
- Unordered list of key value pairs
- Values are indexed by keys
- Keys can be strings or numbers
- Value can be any Python object

Dictionaries

- Creating dictionaries
- Accessing values
- Adding items

```
>>> grades = {'Alice' : 5, 'John' : 4, 'Carl' : 2} 
>>> grades 
{'John': 4, 'Alice': 5, 'Carl': 2}
```

```
>>> grades['John']
4
```

```
>>> grades['Linda'] = 3
>>> grades
{'John': 4, 'Alice': 5, 'Carl': 2,
'Linda': 3}
>>> elements = {}
>>> elements['Fe'] = 26
>>> elements
{'Fe': 26}
```

Variables

- Python variables are always references
- my_list1 and my_list2 are references to the same list
 - Modifying my_list2 changes also my_list1!
- Copy can be made by slicing the whole list

```
>>> my_list1 = [1,2,3,4]
>>> my_list2 = my_list1
```

```
>>> my_list2[0] = 0
>>> my_list1
[0, 2, 3, 4]
```

```
>>> my_list3 = my_list1[:]
>>> my_list3[-1] = 66
>>> my_list1
[0, 2, 3, 4]
>>> my_list3
[0, 2, 3, 66]
```

What is object?

- Object is a software bundle of data (=variables) and related methods
- Data can be accessed directly or only via the methods (=functions) of the object
- In Python, everything is object
- Methods of object are called with the syntax: obj.method
- Methods can modify the data of object or return new objects

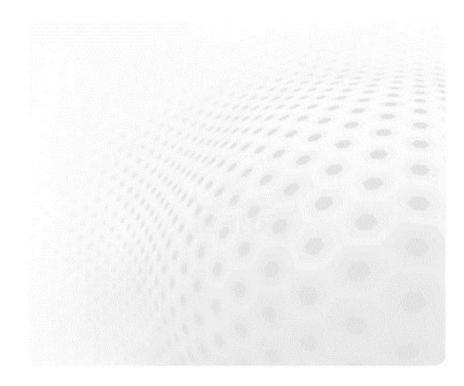
Summary

- Python syntax: code blocks defined by indentation
- Numeric and string datatypes
- Powerful basic data structures:
 - Lists and dictionaries
- Everything is object in Python
- Python variables are always references to objects



Control structures

- if else statements
- while loops
- for loops
- Exceptions



if statement

- if statement allows one to execute code block depending on condition
- code blocks are defined by indentation, standard practice is to use four spaces for indentation

```
example.py
if x > 0:
    x += 1
    y = 4 * x
numbers[2] = x
```

boolean operators:

if statement

there can be multiple branches of conditions

```
if x == 0:
    print "x is zero"
elif x < 0:
    print "x is negative"
elif x > 100000:
    print "x is large"
else:
    print "x is something completely different"
```

Python does not have switch statement

while loop

while loop executes a code block as long as an expression is True

```
x = 0
cubes = {}
cube = 0
while cube < 100:
    cubes[x] = cube
    x += 1
    cube = x**3</pre>
```

for loop

for statement iterates over the items of any sequence (e.g. list)

```
example.py
cars = ['Audi', 'BMW', 'Jaguar', 'Lada']
for car in cars:
    print "Car is ", car
```

- In each pass, the loop variable car gets assigned next value from the sequence
 - Value of loop variable can be any Python object

for loop

- Many sequence-like Python objects support iteration
 - Dictionary: "next" values are dictionary keys

```
prices = {'Audi' : 50, 'BMW' : 70, 'Lada' : 5}

for car in prices:
    print "Car is ", car
    print "Price is ", prices[car]
```

 (later on: file as sequence of lines, "next" value of file object is the next line in the file)

for loop

Items in the sequence can be lists themselves

```
coordinates = [[1.0, 0.0], [0.5, 0.5], [0.0, 1.0]]
for coord in coordinates:
    print "X=", coord[0], "Y=", coord[1]
```

Values can be assigned to multiple loop variables

```
for x, y in coordinates:
    print "X=", x, "Y=", y
```

Dictionary method items() returns list of key-value pairs

```
prices = {'Audi': 50, 'BMW' : 70, 'Lada' : 5}
for car, price in prices.items():
    print "Price of", car, "is", price
```

break & continue

break out of the loop

```
example.py

x = 0
while True:
    x += 1
    cube = x**3
    if cube > 100:
        break

example.py

sum = 0
for p in prices:
    sum += p
    if sum > 100:
        print "too much"
        break
```

continue with the next iteration of loop

```
example.py

x = -5
cube = 0
while cube < 100:
    x += 1
    if x < 0:
    continue
    cube = x**3</pre>
example.py

sum = 0
for p in prices:
    if p > 100:
        continue
    sum += p
```

exceptions

- Exceptions allow the program to handle errors and other "unusual" situations in a flexible and clean way
- Basic concepts:
 - Raising an exception. Exception can be raised by user code or by system
 - Handling an exception. Defines what to do when an exception is raised, typically in user code.
- There can be different exceptions and they can be handled by different code

exceptions in Python

Exception is catched and handled by try - except statements

```
my_list = [3, 4, 5]
try:
    fourth = my_list[4]
except IndexError:
    print "There is no fourth element"
```

User code can also raise an exception

```
if solver not in ['exact', 'jacobi', 'cg']:
    raise RuntimeError('Unsupported solver')
```

List comprehension

- useful Python idiom for creating lists from existing ones without explicit for loops
- creates a new list by performing operations for the elements of list:

newlist = [op(x) for x in oldlist]

```
>>> numbers = range(6)
>>> squares = [x**2 for x in numbers]
>>> squares
[0, 1, 4, 9, 16, 25]
```

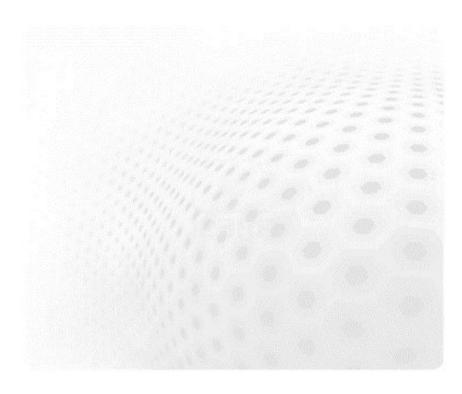
a conditional statement can be included

```
>>> odd_squares = [x**2 for x in numbers if x % 2 == 1]
>>> odd_squares
[1, 9, 25]
```



Functions and modules

- defining functions
- calling functions
- importing modules



Functions

- function is block of code that can be referenced from other parts of the program
- functions have arguments
- functions can return values

Function definition

```
function.py

def add(x, y):
    result = x + y
    return result

u = 3.0
v = 5.0
sum = add(u, v)
```

- name of function is add
- x and y are arguments
- there can be any number of arguments and arguments can be any Python objects
- return value can be any Python object

Keyword arguments

functions can also be called using keyword arguments

```
function.py

def sub(x, y):
    result = x - y
    return result

res1 = sub(3.0, 2.0)
res2 = sub(y=3.0, x=2.0)
```

keyword arguments can improve readability of code

Default arguments

- it is possible to have default values for arguments
- function can then be called with varying number of arguments

```
function.py
def add(x, y=1.0):
    result = x + y
    return result

sum1 = add(0.0, 2.0)
sum2 = add(3.0)
```

Modifying function arguments

as Python variables are always references, function can modify the objects that arguments refer to

```
>>> def switch(mylist):
...     tmp = mylist[-1]
...     mylist[-1] = mylist[0]
...     mylist[0] = tmp
...
>>> l1 = [1,2,3,4,5]
>>> switch(l1)
>>> l1
[5, 2, 3, 4, 1]
```

side effects can be wanted or unwanted

Modules

- modules are extensions that can be imported to Python to provide additional functionality, e.g.
 - new data structures and data types
 - functions
- Python standard library includes several modules
- several third party modules
- user defined modules

Importing modules

import statement

```
example.py
import math
x = math.exp(3.5)
import math as m
x = m.exp(3.5)

from math import exp, pi
x = exp(3.5) + pi

from math import *
x = exp(3.5) + sqrt(pi)

exp = 6.6
from math import *
x = exp + 3.2 # Won't work,
# exp is now a function
```

Creating modules

- it is possible to make imports from own modules
- define a function in file mymodule.py

```
mymodule.py

def incx(x):
    return x+1
```

the function can now be imported in other .py files:

```
import mymodule

y = mymodule.incx(1)

test.py
from mymodule import incx

y = incx(1)
```

Summary

- functions help in reusing frequently used code blocks
- functions can have default and keyword arguments
- additional functionality can be imported from modules



File I/O and text processing

- working with files
- reading and processing file contents
- string formatting and writing to files

Opening and closing files

opening a file:

myfile = open(filename, mode)

- returns a handle to the file

```
>>> fp = open('example.txt', 'r')
>>>
```

Opening and closing files

- file can opened for
 - reading: mode='r' (file has to exist)
 - writing: mode='w' (existing file is truncated)
 - appending: mode='a'
- closing a file
 - myfile.close()

```
example.py
# open file for reading
infile = open('input.dat', 'r')

# open file for writing
outfile = open('output.dat', 'w')

# open file for appending
appfile = open('output.dat', 'a')

# close files
infile.close()
```

Reading from files

a single line can be read from a file with the readline() function

```
>>> infile = open('inp', 'r')
>>> line = infile.readline()
```

it is often convenient to iterate over all the lines in a file

```
>>> infile = open('inp', 'r')
>>> for line in infile:
... # process lines
```

Processing lines

- generally, a line read from a file is just a string
- a string can be split into a list of strings:

```
>>> infile = open('inp', 'r')
>>> for line in infile:
... line = line.split()
```

 fields in a line can be assigned to variables and added to e.g. lists or dictionaries

```
>>> for line in infile:
... line = line.split()
... x, y = float(line[1]), float(line[3])
... coords.append((x,y))
```

Processing lines

sometimes one wants to process only files containing specific tags or substrings

```
>>> for line in infile:
... if "Force" in line:
... line = line.split()
... x, y, z = float(line[1]), float(line[2]), float(line[3])
... forces.append((x,y,z))
```

- other way to check for substrings:
 - str.startswith(), str.endswith()
- Python has also an extensive support for regular expressions in re -module

String formatting

- Output is often wanted in certain format
- The string object has .format method for placing variables within string
- Replacement fields surrounded by {} within the string

```
>>> x, y = 1.6666, 2.33333
print "X is {0} and Y is {1}".format(x, y)
X is 1.6666 and Y is 2.3333
>>> print "Y is {1} and X is {0}".format(x, y)
Y is 2.3333 and X is 1.6666
```

Possible to use also keywords:

```
>>> print "Y is {val_y} and X is {val_x}".format(val_x=x, val_y=y)
Y is 2.3333 and X is 1.6666
```

String formatting

- Presentation of field can be specified with {i:[w][.p][t]}
 - w is optional minimum width
 - .p gives optional precision (=number of decimals)
 - t is the presentation type
- some presentation types
 - s string (normally omitted)
 - d integer decimal
 - f floating point decimal
 - e floating point exponential

```
>>> print "X is {0:6.3f} and Y is {1:6.2f}".format(x, y)
X is 1.667 and Y is 2.33
```

Writing to a file

- data can be written to a file with print statements
- file objects have also a write() function
- the write() does not automatically add a newline

```
outfile = open('out', 'w')
print >> outfile, "Header"
print >> outfile, "{0:6.3f} {0:6.3f}".format(x, y)

outfile = open('out', 'w')
outfile.write("Header\n")
outfile.write("{0:6.3f} {0:6.3f}".format(x, y))
```

file should be closed after writing is finished

Differences between Python 2.X and 3.X

print is a function in 3.X

```
print "The answer is", 2*2 # 2.X
print("The answer is", 2*2) # 3.X

print >>sys.stderr, "fatal error" # 2.X
print("fatal error", file=sys.stderr) # 3.X
```

- in 3.X some dictionary methods return "views" instead of lists.
 - e.g. k = d.keys(); k.sort() does not work,
 use k = sorted(d) instead
- for more details, see http://docs.python.org/release/3.1/whatsnew/3.0.html

Summary

- files are opened and closed with open() and close()
- lines can be read by iterating over the file object
- lines can be split into lists and check for existence of specific substrings
- string formatting operators can be used for obtaining specific output
- file output can be done with print or write()

Useful modules in Python standard library

- math: "non-basic" mathematical operations
- os : operating system services
- glob : Unix-style pathname expansion
- random : generate pseudorandom numbers
- pickle : dump/load Python objects to/from file
- time: timing information and conversions
- xml.dom / xml.sax : XML parsing
- + many more http://docs.python.org/library/

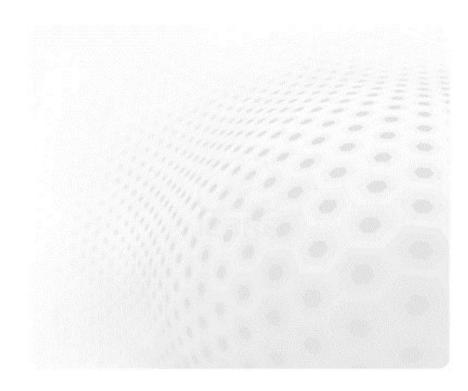
Summary

- Python is dynamic programming language
- flexible basic data structures
- standard control structures
- modular programs with functions and modules
- simple and powerful test processing and file I/O
- rich standard library



Object oriented programming with Python

- Basic concepts
- Classes in Python
- Inheritance
- Special methods



OOP concepts

- OOP is programming paradigm
 - data and functionality are wrapped inside of an "object"
 - Objects provide methods which operate on (the data of) the object
- Encapsulation
 - User accesses objects only through methods
 - Organization of data inside the object is hidden from the user

Examples

- String as an object
 - Data is the contents of string
 - Methods could be lower/uppercasing the string
- Two dimensional vector
 - Data is the x and y components
 - Method could be the norm of vector

OOP in Python

- In Python everything is a object
- Example: open function returns a file object
 - data includes e.g. the name of the file

```
>>> f = open('foo', 'w')
>>> f.name
'foo'
```

- methods of the file object referred by f are f.read(),
 f.readlines(), f.close(), ...
- Also lists and dictionaries are objects (with some special syntax)

OOP concepts

class

- defines the object, i.e. the data and the methods belonging to the object
- there is only single definition for given object type

instance

- there can be several instances of the object
- each instance can have different data, but the methods are the same

Class definition in Python

- When defining class methods in Python the first argument to method is always self
- self refers to the particular instance of the class
- self is not included when calling the class method
- Data of the particular instance is handled with self

```
class Student:
    def set_name(self, name):
        self.name = name

    def say_hello(self):
        print "Hello, my name is ", self.name
```

Class definition in Python

```
class Student:
    def set_name(self, name):
        self.name = name
    def say_hello(self):
        print "Hello, my name is ", self.name

# creating an instance of student
stu = Student()
# calling a method of class
stu.set_name('Jussi')
# creating another instance of student
stu2 = Student()
stu2.set_name('Martti')
# the two instances contain different data
stu.say_hello()
stu2.say_hello()
```

Passing data to object

- Data can be passed to an object at the point of creation by defining a special method __init__
- __init__ is always called when creating the instance

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

In Python, one can also refer directly to data attributes

```
>>> from students import Student
>>> stu1 = Student('Jussi')
>>> stu2 = Student('Martti')
>>> print stu1.name, stu2.name
'Jussi', 'Martti'
```

Python classes as data containers

 classes can be used for C-struct or Fortran-Type like data structures

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

instances can be used as items in e.g. lists

```
>>> stu1 = Student('Jussi', 27)
>>> stu2 = Student('Martti', 25)
>>> student_list = [stu1, stu2]
>>> print student_list[1].age
```

Encapsulation in Python

- Generally, OOP favours separation of internal data structures and implementation from the interface
- In some programming languages attributes and methods can be defined to be accessible only from other methods of the object.
- In Python, everything is public. Leading underscore in a method name can be used to suggest "privacy" for the user

Inheritance

- New classes can be derived from existing ones by inheritance
- The derived class "inherits" the attributes and methods of parent
- The derived class can define new methods
- The derived class can override existing methods

Inheriting classes in Python

```
class Student:
...
class PhDStudent(Student):
    # override __init__ but use __init__ of base class!
    def __init__(self, name, age, thesis_project):
        self.thesis = thesis_project
        Student.__init__(self, name, age)

# define a new method
    def get_thesis_project(self):
        return self.thesis

stu = PhDStudent('Pekka', 20, 'Theory of everything')
# use a method from the base class
stu.say_hello()
# use a new method
proj = stu.get_thesis_project()
```

Special methods

- class can define methods with special names to implement operations by special syntax (operator overloading)
- Examples
 - __add__, __sub__, __mul__, __div__
 - for arithmetic operations (+, -, *, /)
 - __cmp__ for comparisons, e.g. sorting
 - __setitem__, __getitem__ for list/dictionary like syntax using []

Special methods

```
class Vector:
    def __init__(self, x, y):
        self.x = x
        self.y = y

    def __add__(self, other):
        new_x = self.x + other.x
        new_y = self.y + other.y
        return Vector(new_x, new_y)

v1 = Vector(2, 4)
v2 = vector(-3, 6)
v3 = v1 + v2
```

Summary

- Objects contain both data and functionality
- class is the definition of the object
- instance is a particular realization of object
- class can be inherited from other class
- Python provides a comprehensive support for object oriented programming ("Everything is an object")