Course March 2022

Molecular
Electronic
Structure
Group

Lectures in software design in python

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Introduction

Why Programming (software) design?

Readability

Understandable
by others (and you)

Maintainability

Fixing bugs

Upgrade to new
environments

Extensibility/flexibility

Add new
features

Do not waste your time!

Introduction

Readability

- You may want to reuse your code in the future
- You may want to share your code
- You will to explain how to use your code to others
- You will not have much time to read your code
- You may not remember how your code works anymore

Make your code readable!

Introduction

Maintainability

- Your OS will become obsolete
- Your Python version will become obsolete
- Your computer will become obsolete
- You will not have time to update your code
- You may not remember how your code works anymore

Make your code intuitive!

Introduction

Extensibility

- You may want to add new features to your code
- These features may conflict with your current structure
- You will not have time to change your code strucuture
- You may not remember how your code works anymore

Make your code flexible!

Introduction

The truth

- Your code (design) is crap: no users (maybe you in recent future)
- Your code is bad: future you is your only user
- Your code is fine: future you is your main user
- Your code is good: future you among some other researchers are users
- Your code is great: many researchers in your field may be users (future you included)

This is also for you!

Introduction

Like writing a paper!

What is a good design?

- **Logical and intuitive**
  People do not like to read manuals (and probably neither do you)
- **Less comments and better code**
  let the code speak for you
- **Divide and conquer**
  Properly organize you code in files, modules, functions, paragraphs,..
- **Explicit better than implicit (but..)**
  Simple and long better than short (compact) and complicated
- **(…) Make use of available good python modules**
  do not reinvent the wheel. Better notation is always nice!

Logical and intuitive

How?

- **Use conventions to write: PEP8**
  - ***variable names:***
    explicit names, lower case, spaces as underscore “_”
  - ***blank lines and spaces:***
    use them to separate logical blocks in your code
- **Aim for a good equation-code correspondence**
  write helper functions if necessary
- **Let the code guide the structure**
  minimize module imports by playing with scopes

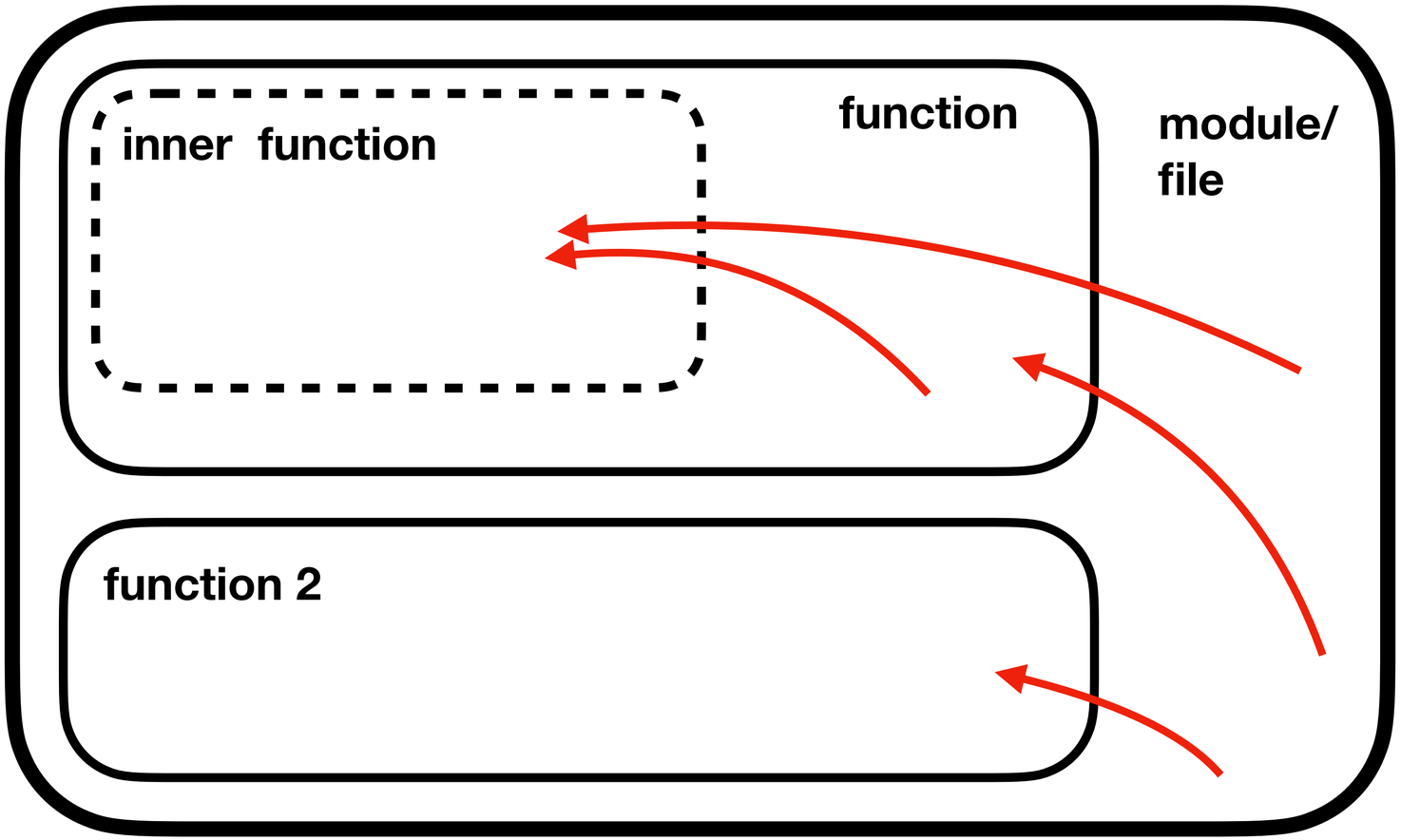
Example 1

Some initial advices

- **Use good code editor (IDE):**
  PyCharm, Visual studio, Spider, etc..
- **Get used to a version control system (VCS) —> git**
  very easy to use through IDE
- **Check the documentation (or StackOverflow)**
  do your research before coding
- **Prioritize standard library**
  over other obscure modules
- **Try to use widely compatible syntax**
  support old versions of Python

Example 2

Variable Scope



Example 3

Generators/Iterators

generator  **Interator**

```
def generator(n):
    for i in range(n):
        sum1 = 0
        for j in range(5):
            sum1 += i ** 2 + j

        yield sum
```

```
for element in generator(10):
     print(element)
```

- **iteration variables generated on the fly**
- **Memory efficient**

Example 4

Fortran/C vs Python

FORTRAN/C

- Small set of instructions
- Simple instructions very flexible
- Short documentation, lots of creativity
- Fast and insecure
- Compiled
- Not so nice syntax
- Fewer external libraries and not so easy to use

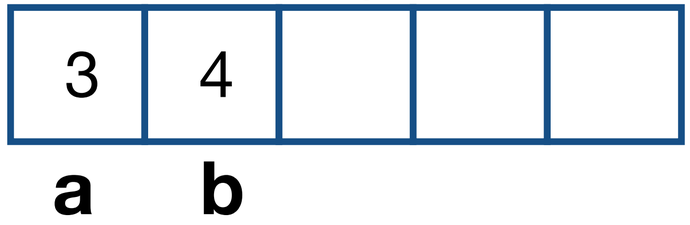
Python

- Large set of instructions
- Complex instructions and very specific
- Long documentation, lots of research (and creativity)
- Slow and safe
- Interpreted
- Nice syntax
- Lots of external libraries easy to use

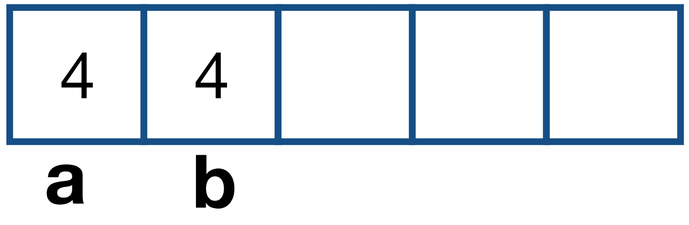
Fortran/C vs Python

Memory structure in Fortran/C

RAM Memory



RAM Memory

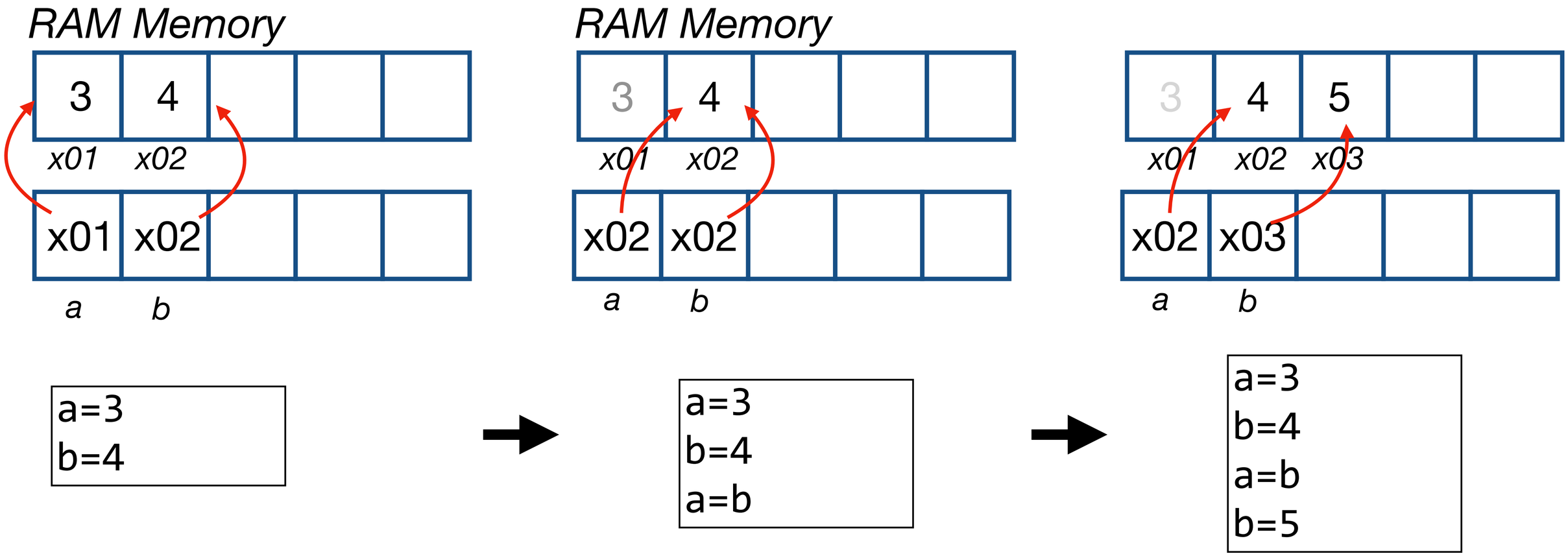



```
a=3
b=4
```

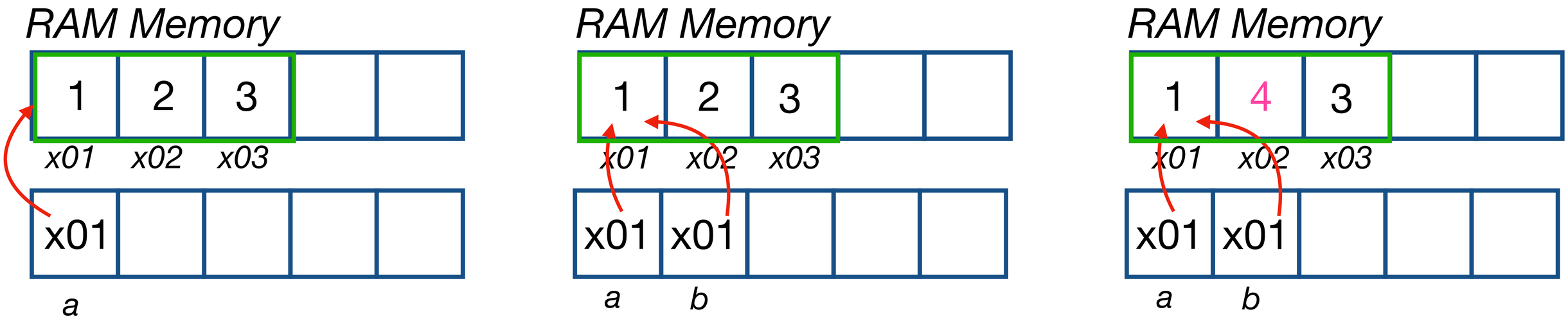
```
a=3
b=4
a=b
```

Fortran/C vs Python

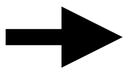
Memory structure in Python



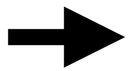
Fortran/C vs Python




```
a=[1, 2, 3]
```



```
a=[1, 2, 3]
b=a
```



```
a=[1, 2, 3]
b=a
b[1] = 4
```

In Python everything is an object!

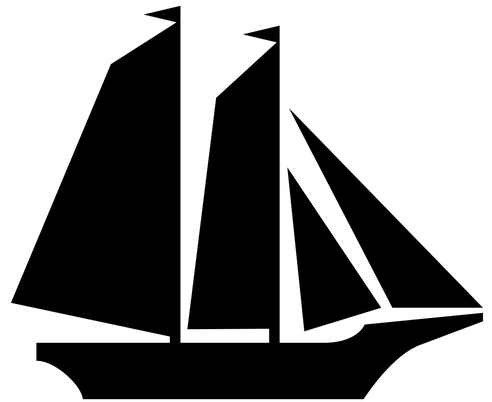
Objects in Python

Object: Structured variable

```
object.method()

object.variable
```

- **Internal variables (internal state)**
  Determine the properties of an object
- **Methods**
  functions than act on the internal state
  - *Modifiers*
    Modify the state of the object
  - *Informatives*
    Return data based on the state of the object

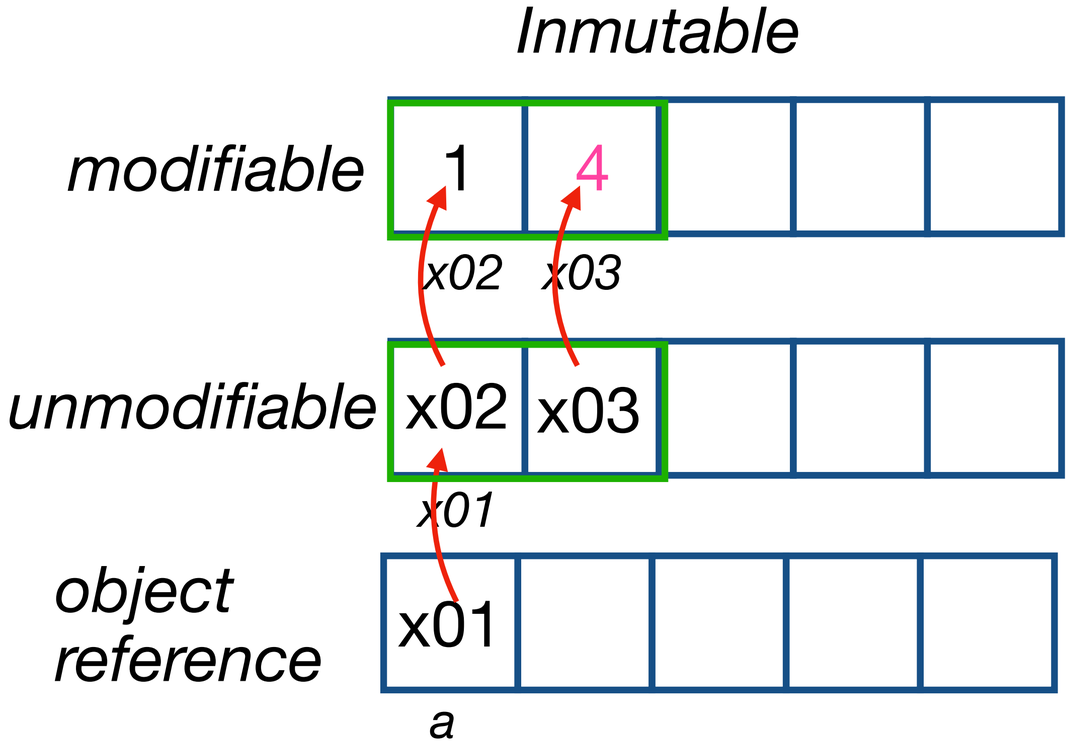


Objects in Python

types of objects: *a security measure*

- **mutable**
  can modify its contents
- **Inmutable**
  cannot modify its contents

Warning! an inmutable object can contain mutable contents



Objects in Python

Custom objects

Class

Contains the blueprints
to generate an object

Instance of a class

Object itself created
from a class

Example:

The blueprints of a ship
(Blueprint type object)

The ship called “Titan”
(ship type object)

Objects in Python

Getter/setter methods

- **getter**
  get data from inner variables (get property)
- **setter**
  set data to inner variables (modify object)

```
object.get_data()
object.set_data(data)
```

Private/public methods

- **Private**
  method used only in the same object (_)
- **Public**
  general methods

```
object._get_method()
object._set_method(data)
```

Example 5

Core design

Programming strategies

Top down

Usual in high level languages

Usual in low level languages

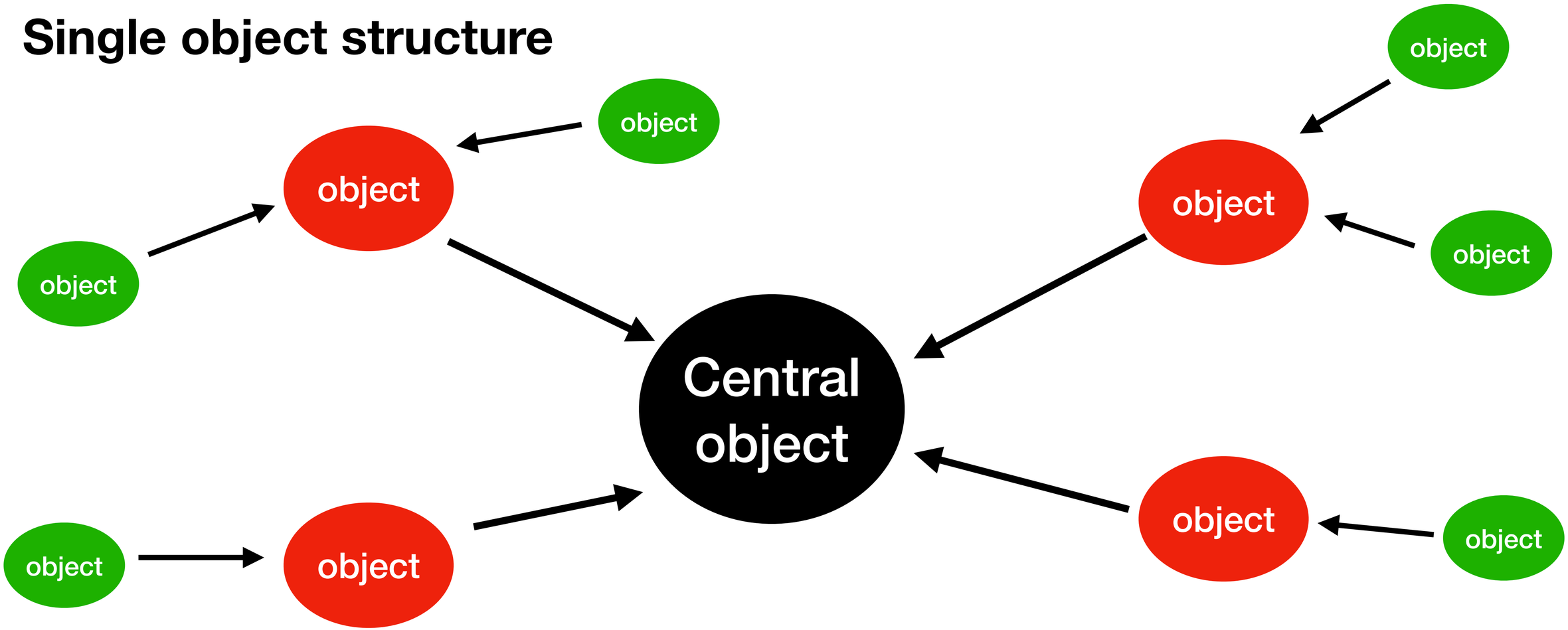
Bottom up

Low level languages

Example 6

Core design (object oriented)

Single object structure



Core design (object oriented)

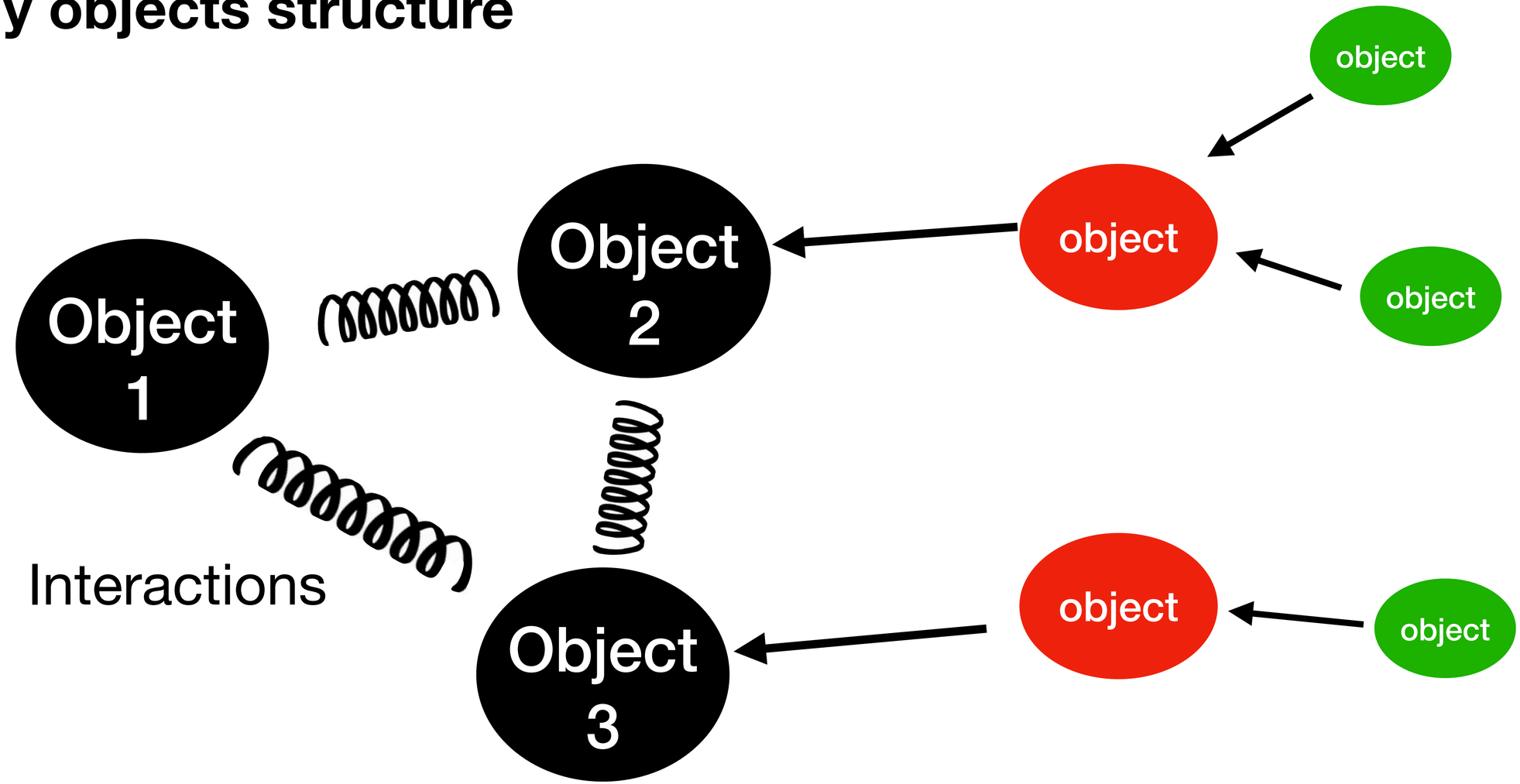
Single object structure

- Data collection (from file/terminal/..)
- Object creation (using data)
- Object modification
- Data extraction (from object)
- Data presentation

Example 7a

Core design (object oriented)

Many objects structure



Core design (object oriented)

Many objects structure

through **Functions**

Multiple objects as arguments

```
data = interaction_function(object_1, object_2):
print(data)
```

Multiple objects and other arguments

through **Operators**

Two objects operate

```
data = object_1 * object_2
print(data)
```

Only two objects, no arguments

Core design (object oriented)

Several interesting operators

- addition
- product
- length
- string representation
- get item
- iterator
- equal

```
self.__add__(self, other)
self.__radd__(self, other)


self.__len__(self)
self.__str__(self)
self.__getitem__(self)
self.__iter__(self)
self.__eq__(self, other)
```

Core design (object oriented)

Multiple object structure

- Data collection (from file/terminal/..)
- Objects initialization (using data)
- Objects interaction
- Data extraction (from final objects/functions)
- Data presentation

Example 7b/8

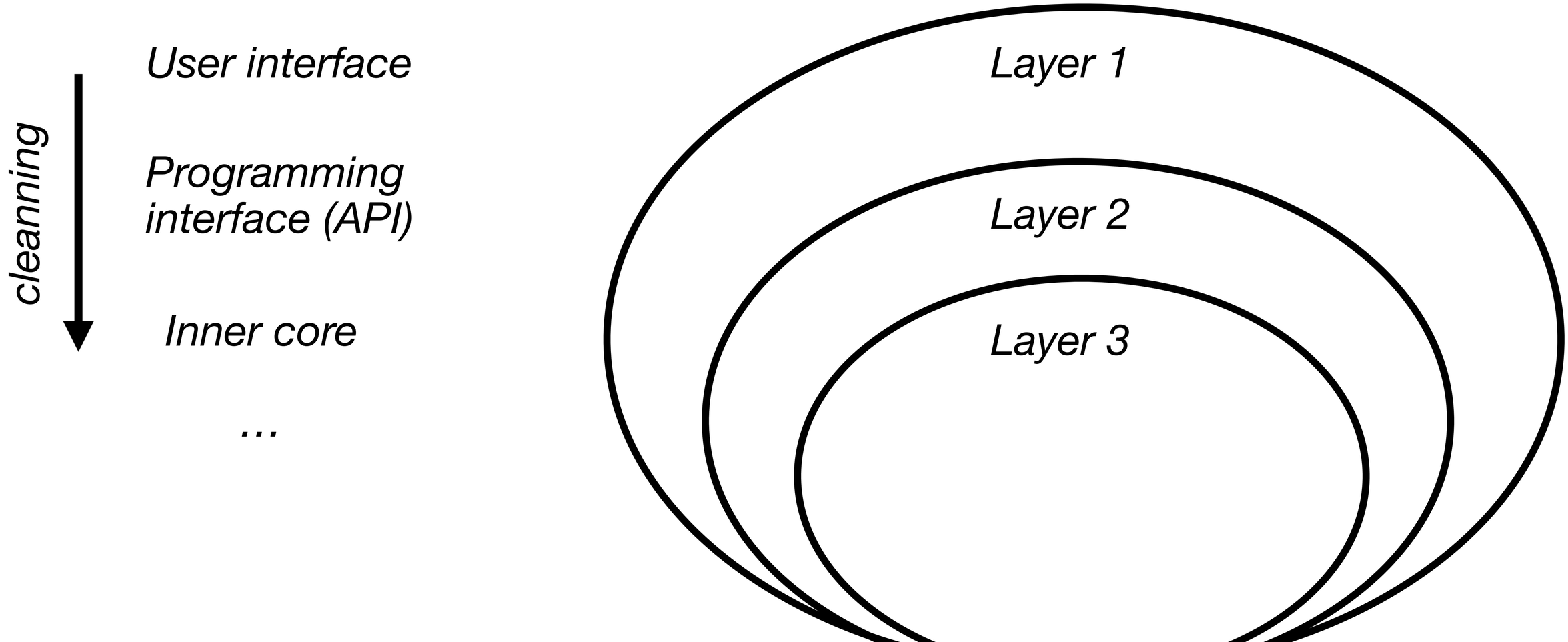
Code upgrade

Maintainability and extensibility

- **Abstraction**
  Relation between real objects and Python objects
- **Encapsulation**
  Separate the code in self contained parts
- **Polymorphism**
  Objects mimic behavior of other objects

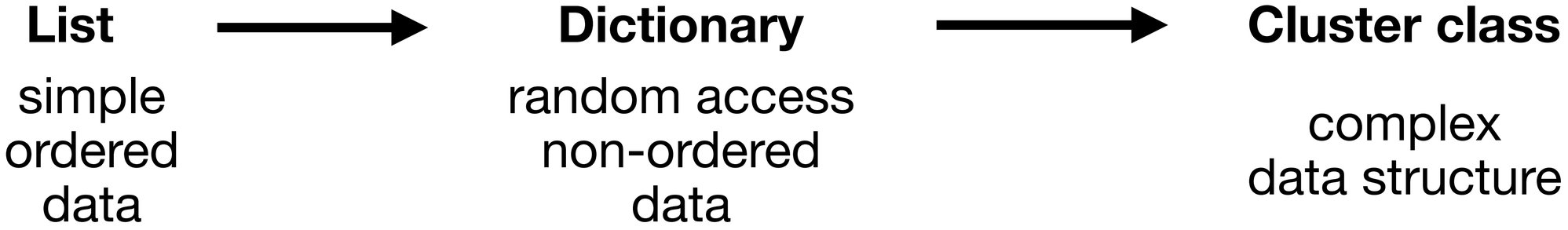
Code upgrade

working in the code



Code upgrade

natural upgrade paths



Example 9

Code upgrade

upgrade file structure

```
root
├─main.py
└─fileio.py          module
```

main.py

```
from fileio import my_funct
```

```
root
├─main.py
└─fileio  module
  ├─ __init__.py
  └─ support.py
```

__init__.py

```
from support import my_funct
```

Example 10

User interfaces

- **GUI (graphical interface): wxWidgets, Tkinter, QT**
  Based on windows, buttons, bars, etc..

- **Text menu interface:**
  Interactive numbered menu items

- **Command line tools: argparse**
  Unix-like scripts executed in the console

Example 11

Error handling

- **Try / except clause**

```
try:
    Some code that produces error

except Error:
    handling error code
```

- **raise Error**

```
try:
    raise SomeError
except SomeError:
    handling error code
```

Example 12