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

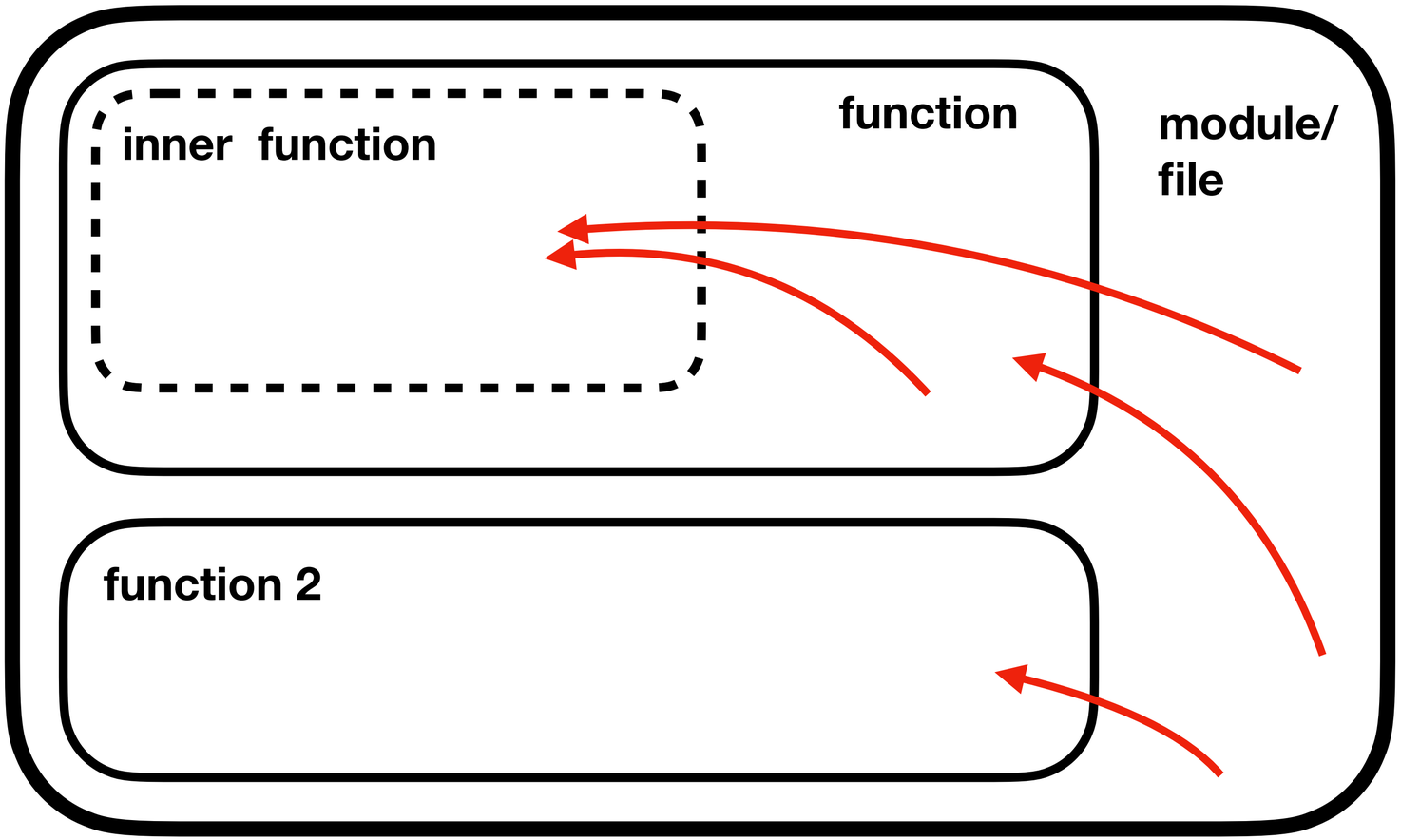
Example 1

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

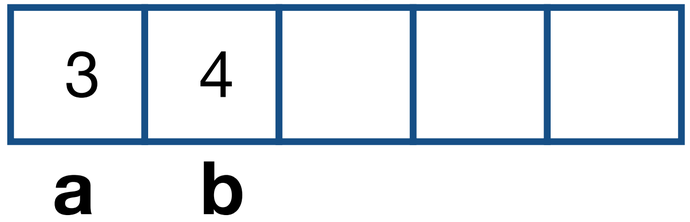
Variable Scope



Example 3

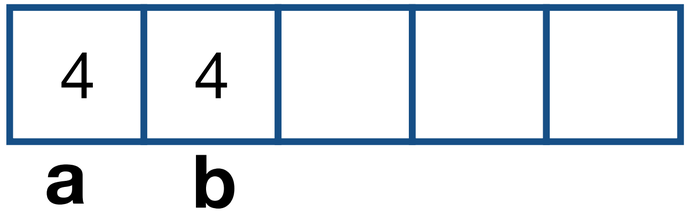
Fortran/C vs Python

RAM Memory




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

RAM Memory




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

Fortran/C vs Python

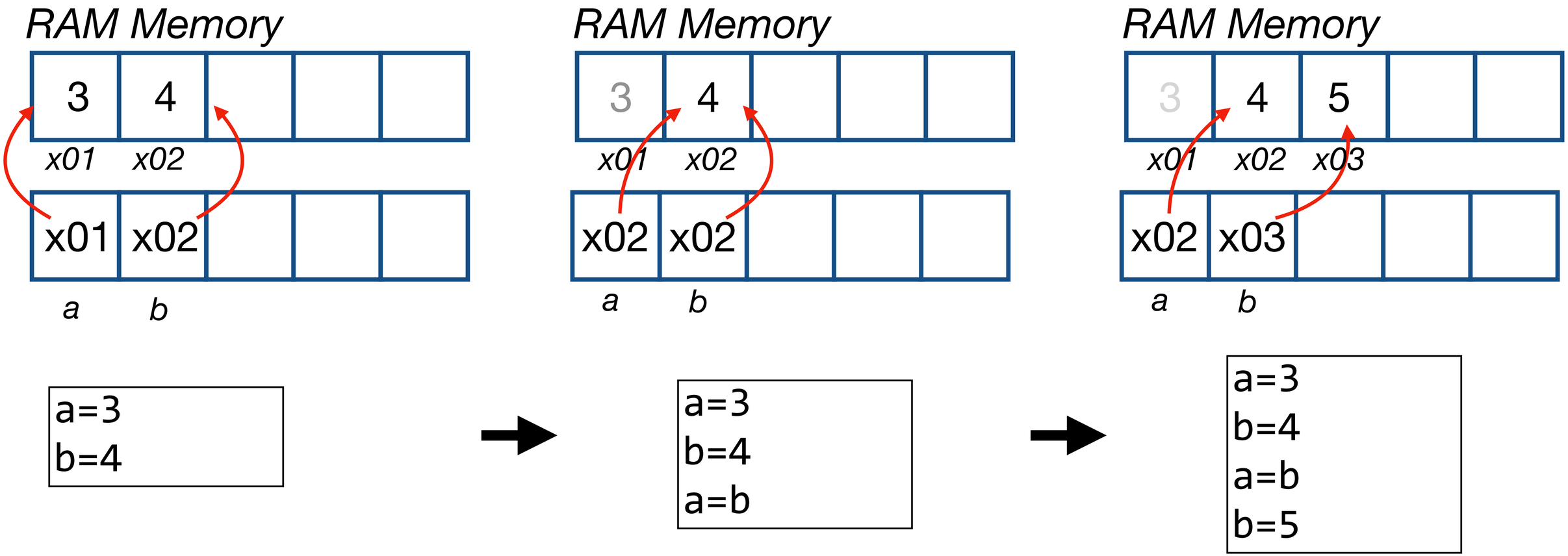
FORTRAN/C

- 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

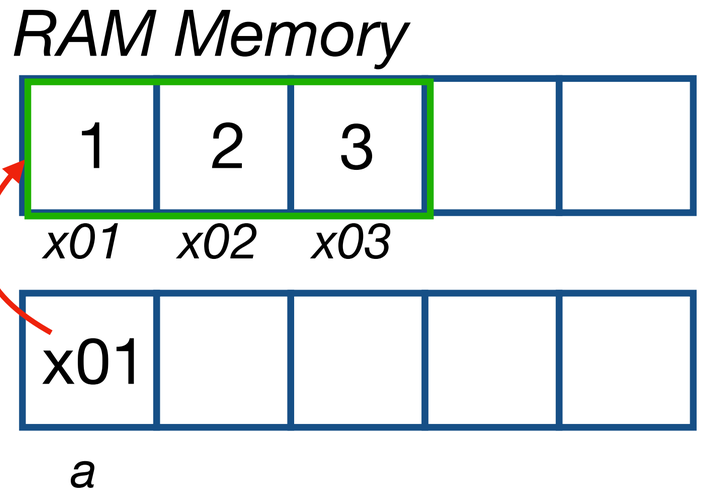
Python

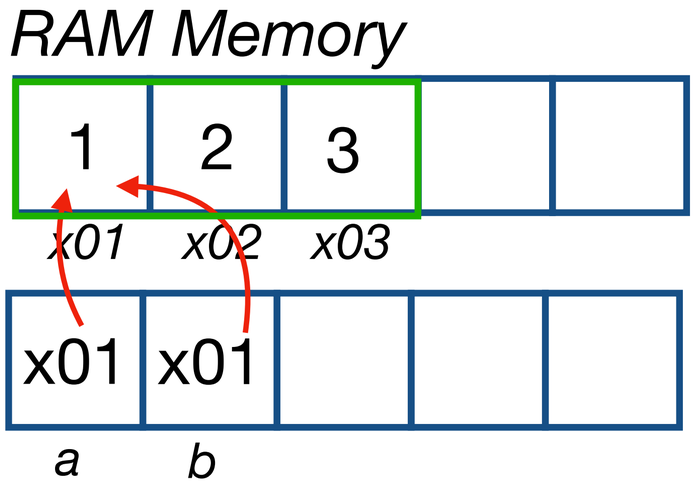
- Large set of instructions
- Complex instructions and very specific
- Long documentation, lots of research (and creativity)
- Slow and safe
- Interpreted
- Nice syntax
- Lots of external libraries easy to use

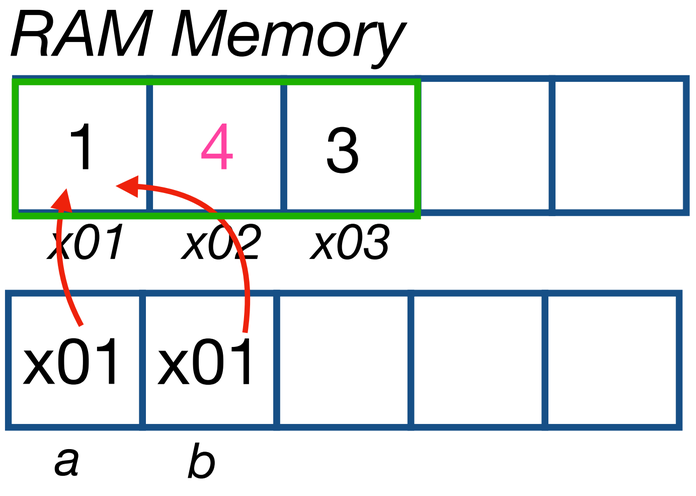
Fortran/C vs Python



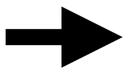
Fortran/C vs Python



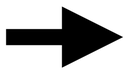





```
a=[1, 2, 3]
```



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



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