

Center for Individual Nanoparticle Functionality

- Introduction
- What is a computer program
- Math
- Types
- Variables
- Containers
- Loops
- Boolean expressions
- Control flow (if-elif-else)
- Functions
- Summary

Python part 0



Center for Individual Nanoparticle Functionality

- Introduction

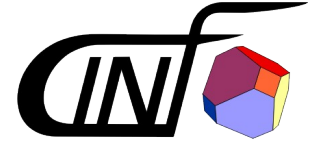
Python part 0

The program



- Move through each of the topics in the outline
- For each topic there will be:
 - A presentation by me
 - A “type along” session, where we type the new things together
 - A few exerciser (the exercises are meant mainly for typing repetition, so most are simple)
- There will also be a few short detours along the way

Why program? To do cool stuff



- To do data treatment (reproducably)
- Talk to equipment - to use it for things that the manufacturer did not think of
- To combine data from different sources
- To produce good looking graphs
- To automate tedious and/or time consuming tasks
- And because its fun – programming is like Lego for adults

Why program? For reproducibility



- As scientists we often rely need to:
 - Repeat the same data treatment for different data sets
 - Repeat a procedure
 - Repeat repeat repeat
- But people are not very good at repeating simple tasks (they get bored or forget)
- Computers on the hand are **great** at repeating
- Why not let them do it

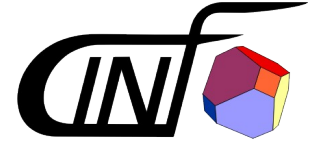
The “super coder” myth



- That programming skills are somehow special and something that only people with a predeposition can do
- That skills are distributed in a bimodal fashion with only super-ninjas and those that cannot not at all

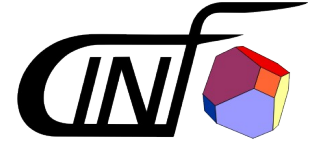
FALSE!

The “super coder” myth is bogus



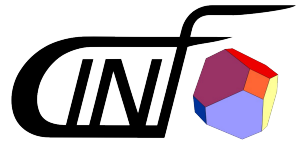
- Programming is a skill just like any other and anyone can develop along the skill levels
- It takes teaching, repetition and practice, just like any other skill
- Relax, enjoy learning something new and don't panic, if you do not feel able to program facebook from scratch by the end of the day
- **That's normal!**

A bit about wording



- I have chosen to be accurate with wording
- Might seem a little abstract
- E.g:
 - **Object** An object “is a thing” in a program
 - **Sequence** A sequence is “a string of somethings”
 - etc.

- Will use Python
 - Ease of use
 - Emphasis on readability
 - Popularity in the scientific community
- MANY or all of the concepts we talk about are general and used in many programming environments



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Python part 0

What is a computer program



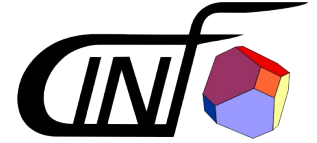
- A set of instructions
- Executed in order
- Needs to be correct, follow a syntax
- Think of it like ...
- A cooking recipe
- Give a chef instructions one at a time

Directions

- 1. In a large bowl, sift together the flour, baking powder, salt and sugar. Make a well in the center and pour in the milk, egg and melted butter; mix until smooth.
- 2. Heat a lightly oiled griddle or frying pan over medium high heat. Pour or scoop the batter onto the griddle, using approximately 1/4 cup for each pancake. Brown on both sides and serve hot.

<http://allrecipes.com/recipe/good-old-fashioned-pancakes/>

What is a computer program



with sift:

- apply flour

- apply baking powder

- apply salt

- apply sugar

make center well

apply egg

apply milk

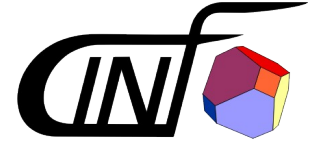
apply melted butter

while not well mixed:

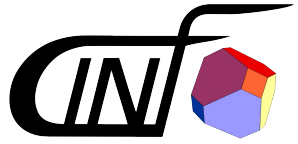
- mix with spoon

Pseudo-code to make pancake
batter. Yum!

The interpreter



- Usually programs are written as sequences of instructions in a file
- In Python (unlike all languages) you actually can give it instructions *live*
- For this you use the “*the interpreter*”
- Usually used to experiment or test
- We will use it to learn interactively



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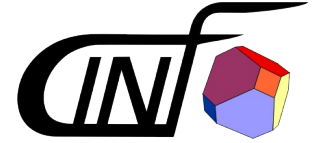
- What is a computer program
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Python part 0

- All the usual suspects
- Except division, may not do what you want
- Order of operations as you would expect

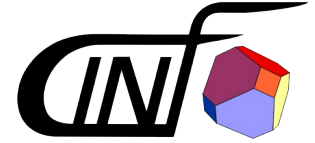
PEMDAS

Operator	Action
+	Plus
-	Minus
/	Division (careful)
*	Multiplication
**	Raise to power
()	Used for precedence



- With division `/` between integers performs flooring integer division
 - e.g. $3/4=0$
- To turn it into float, convert one to float first
 - $\text{float}(3)/4 = 0.75$
- Can use exponential notation
$$4\text{E}-8 = 4 * 10^{-8}$$
- Let's get started typing

Start the Python interpreter



Start the Python interpreter from your program menu

First "instruction"

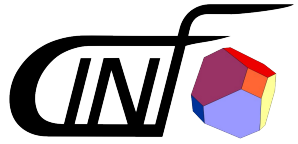
The Python version

>>> Indicates a prompt
i.e. "enter stuff here"

Result of
first "instruction"

```
Python 2.7.6 (default, Mar 22 2014, 22:59:56)
[GCC 4.8.2] on linux2
Type "help", "copyright", "credits" or "license" for more information.
>>> print "Hello World"
Hello World
>>> 2 + 4
6
>>> 
```

Type along session in the terminal:
Math

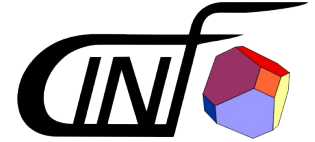


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Python part 0

Types



- In computer programs, items (called objects) have **a type**
- The type determines:
 - What data it can contain
 - How it interacts with other objects of the same or a different type
 - In short, what you can do with it
 - (If it can be changed)
- In short, an objects type defines its functionality



Type: Shoe

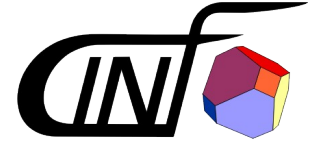


Type: Box



Type: Integer

Types



- You have already met a few types
- The most fundamental are:

float is short for floating point number and is the universal representation for fractional numbers in science.

Also sometimes referred to as
single → single precision float
double → double precision float

Type	Example
int	47
float	47.0
string	"fourtyseven"
bool	True
NoneType	None

This one we haven't seen before. It means:
"nothing to see here"

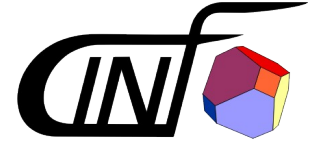
The *type* function



- The *type* function can be used to get the type of an object

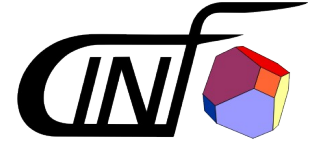
```
>>> type(47)
<type 'int'>
>>> type(47.0)
<type 'float'>
>>> type('fourtyseven')
<type 'str'>
>>> type(True)
<type 'bool'>
```

Wait, what is a function?



- A function gathers useful and re-useable bits of work together
- A function:
 - Takes input and produces output (just like in math)
 - And/or can perform tasks
- The different inputs to a function are called *“arguments”*
- Functions can be *“called”* or *“invoked”*
- Function can *“be given”* or *“passed”* arguments

The anatomy of a function call



open parenthesis close parenthesis

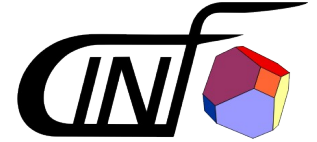
function name arguments

```
>>> type(1.0)
<type 'float'>
```

type is a function that "takes" one argument
we are "calling" **type** with the argument 1.0
we can "pass" any Python object to **type**

https://openhatch.org/wiki/Boston_Python_Workshop_8/Friday/Tutorial#Types

Type along session in the terminal:
Types



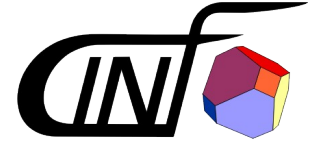
- Get the type of different objects with **type()**
- Try math on objects that you would not expect to work
 - E.g. multiply a strings, booleans and numbers
 - Does it work?
 - What is the type
 - Is there a logic to it?

The command history



- Try and press the up arrow in the interpreter
- The interpreter keeps a history of what you have entered
- Makes it easy to go back and repeat actions
- Simple press *up arrow* untill the correct command and then *enter*

Working with strings



- Strings are fundamental (also for scientists)
- 'This is a string'
- To concatenate strings use +
- To add the string representation of an object to a string, use `str(object)`
- ' and " are synonymous
- The used quote needs to be escaped inside the strings

Working with strings

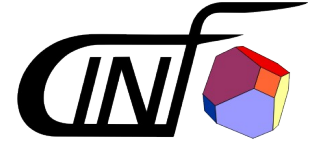


```
>>> 'The start ' + 'and the end'  
'The start and the end'
```

```
>>> 'Concatenating a number to the string ' +  
str(1)  
'Concatenating a number to the string 1'
```

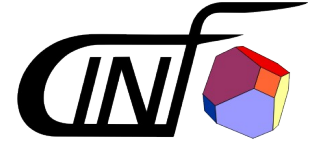
```
>>> 'It\'s necessary to quote'  
"It's necessary to quote"
```

```
>>> "It's necessary to quote"  
"It's necessary to quote"
```



Type along session in the terminal:
Types

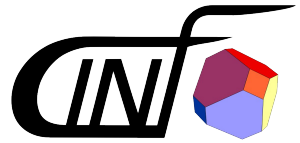
Strings - Exercises



- Exercise 1-4 on

<http://www.codecademy.com/courses/python-beginner-en-kSQwt/0/1>

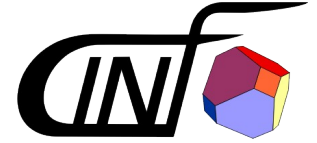
(Keep this page open for later)



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Python part 0



- A variable **is a nametag** for an object
- Almost like math variables
- Can “be” of **any type**
- Giving an object a name is called *assignment*

```
>>> x = 47
>>> x
47
>>> type(x)
<type 'int'>
>>> 2 * x
94
```

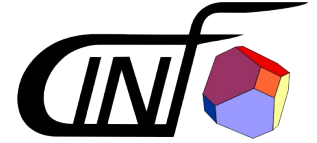
Mix and match, variables and object



- You can mix variables with objects in expression
- Think of it as if variables are replaced by the object they refer to

```
>>> a = 22
>>> b = 2
>>> the_answer = 2 * a - b
>>> the_answer
42
```

Assignment to a variable

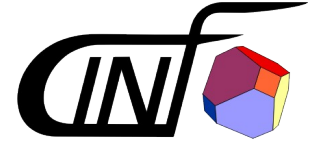


- What happens if you try and assign a variable to a variable?

`a = 47`

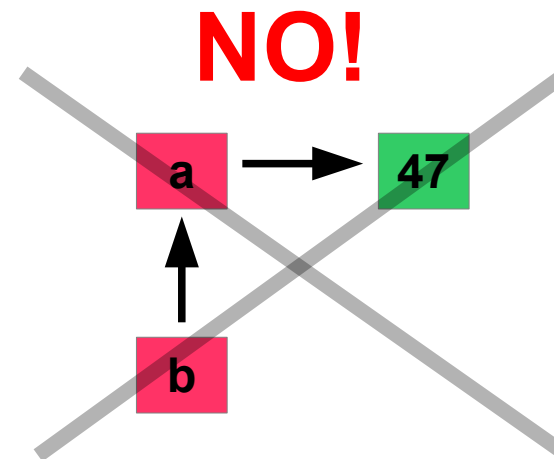
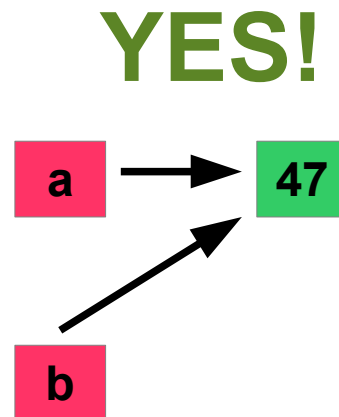
`b = a`

Assignment *to* a variable



- You ***cannot*** assign a variable to another variable
- It will fall through and point to the same object

```
>>> a = 47  
>>> b = a
```

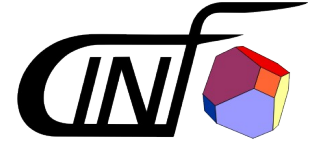


Variables



- Variable names can only contain letters and underscores (no spaces)
- Keep consistent, use lowercase underscore
 - measurements
 - measurement_set
 - number_of_measurements
- Must be descriptive, to help yourself read your program
 - Yes: number_of_points, length_of_queue etc.
 - No: number, length, size, my_integer etc.

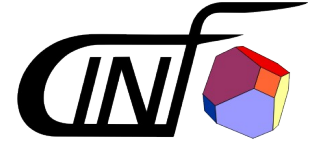
About output



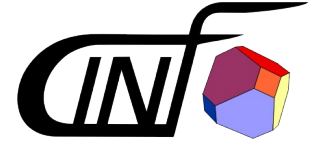
- About of an expression will be printed to screen ...
- ... unless assigned to a variable
- Functions can **both change the value of something that you pass in and return it**

```
>>> 4
4
>>> a = 4
>>> a
4
```

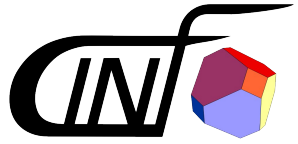
Variables – Type along



Type along session in the terminal:
Variables



- Assign objects of different types to variables
- Try expressions with variables only
- Try expressions with a combination of variables and objects
- Assign a number to a variable ($a=47$),
 - assign a new variable to that first variable ($b=a$)
 - check the value of a and b
 - change the value of a
 - check the value of a and b

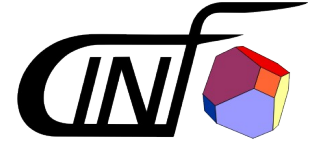


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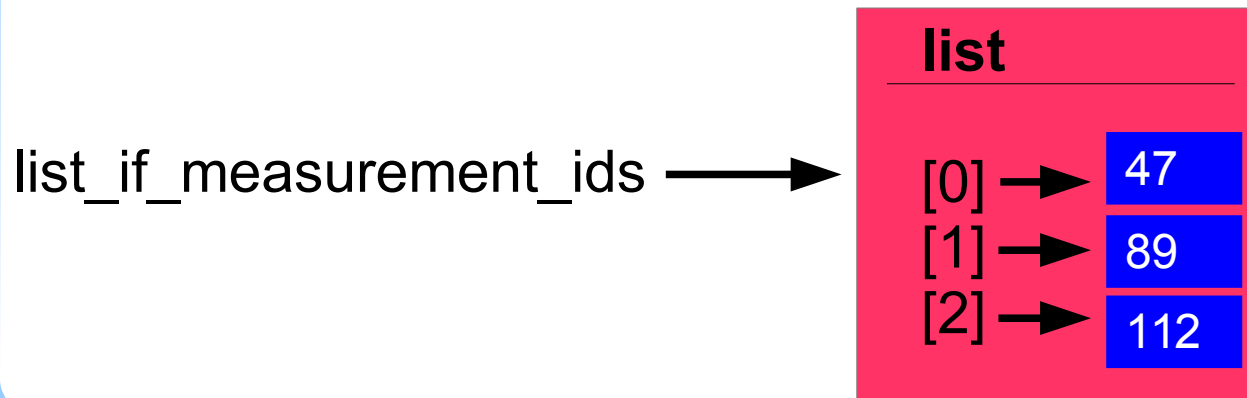
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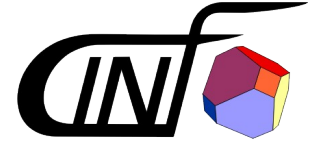
Containers



- Creating a variable for every measure that you need is impractical
- Containers can **contain** several objects and make it easy to access them
- Containers are in themselves objects that a variable can point to

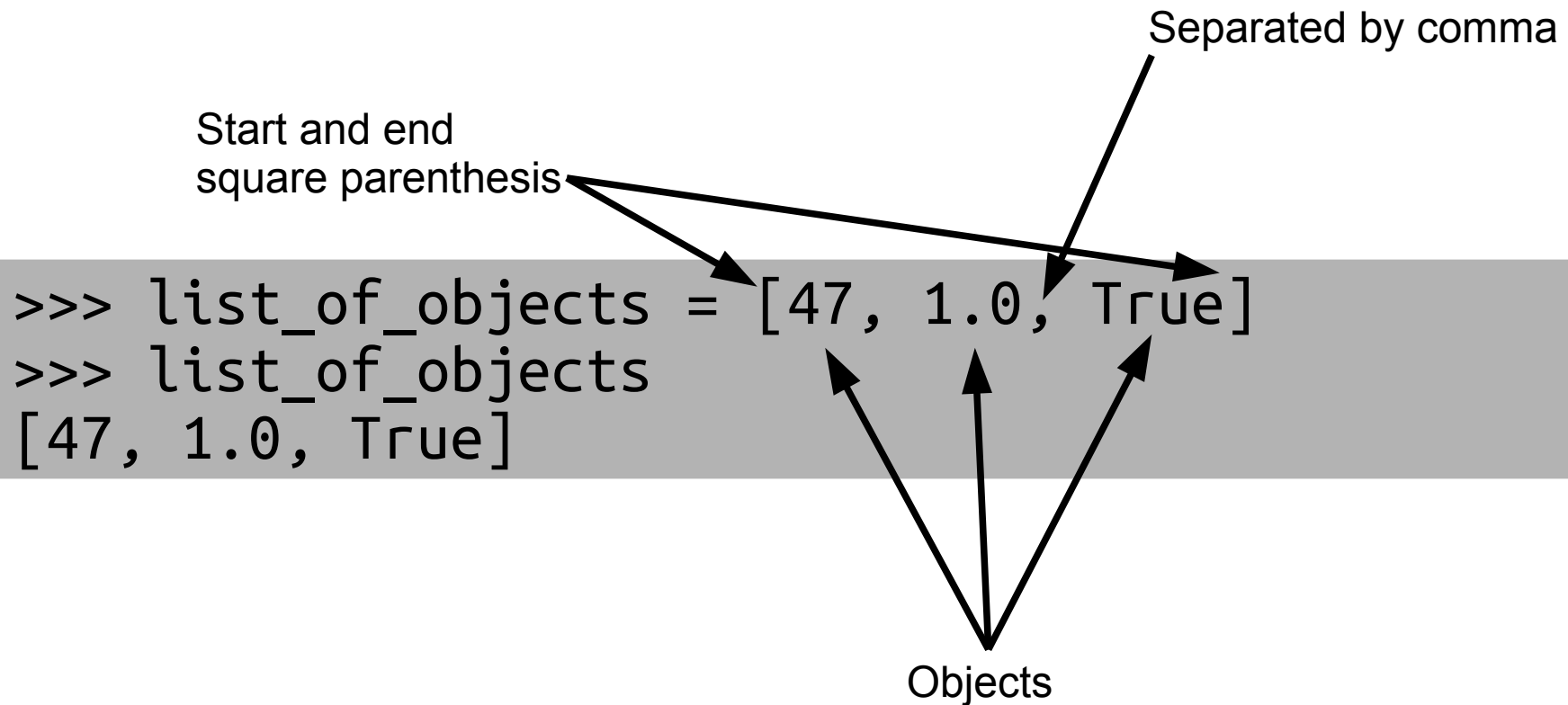
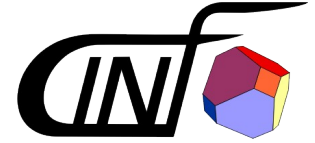


The simplest container – the **list**



- **Ordered:** Objects are in order in *slots*
- **In-homogeneous:** A list can contain a mix of different types of objects
- Objects are assigned and retrieved with integer indices
- Create a list by typing `[]` or calling `list()` on a sequence

A list



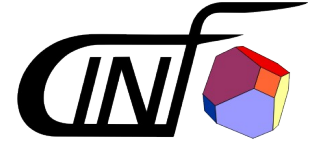
Indexing lists



- To index a list use the [*index_number*]
- Index numbers are 0-based (first one is 0)

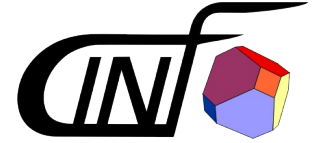
```
>>> list_of_objects = [47, 1.0, True]
>>> list_of_objects[0]
47
>>> list_of_objects[2]
True
>>> list_of_objects[0] = 7
>>> list_of_objects
[7, 1.0, True]
```

List – Type along



Type along session in the terminal:
List

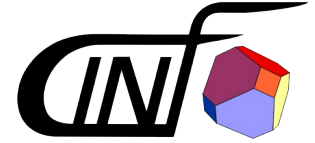
Add elements in a list



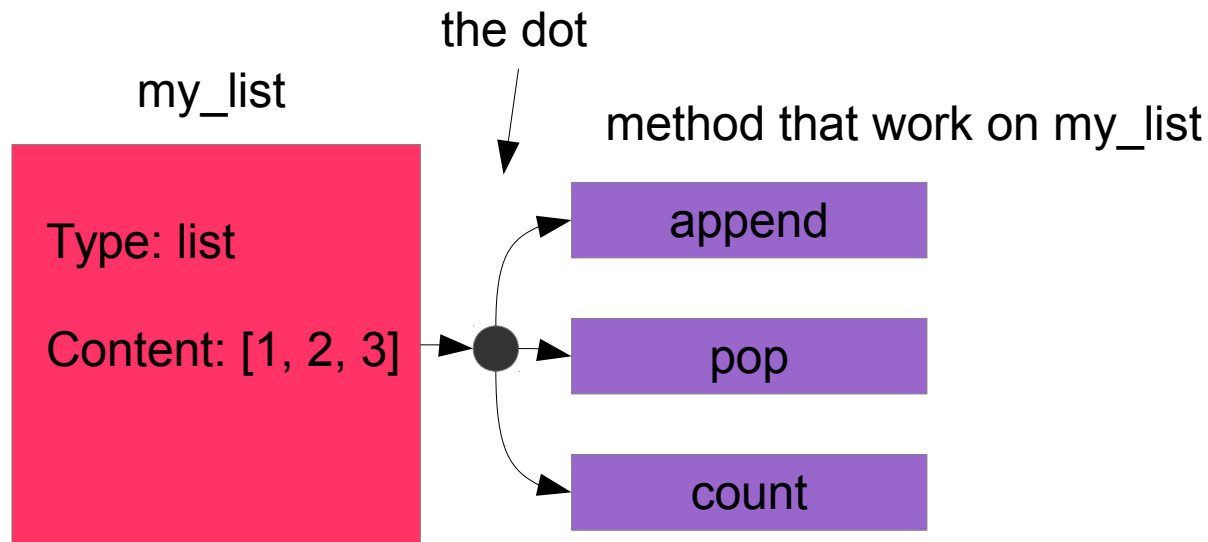
- Primarily with *append*

```
>>> list_of_objects  
[7, 1.0, True]  
  
>>> list_of_objects.append(9)  
>>> list_of_objects  
[7, 1.0, True, 9]
```

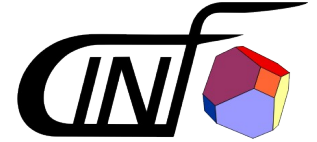

Hold on, what is a method?



- A method is a functions that:
 - Is attached to an object
 - Performs actions on this object
- All objects have methods, even ints

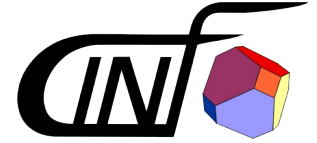


A list has quite a few methods



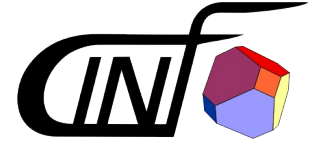
- Call the *dir* function of an object to find its methods
- **append** adds an object to the end
- **count** counts occurrences of an object
- **index** returns first index of an object
- **insert** insert object at index
- **remove** removes first occurrence of object
- **pop** remove and return from index
- ... more

List – Type along



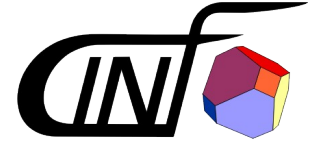
Type along session in the terminal:
List

List - Exercises

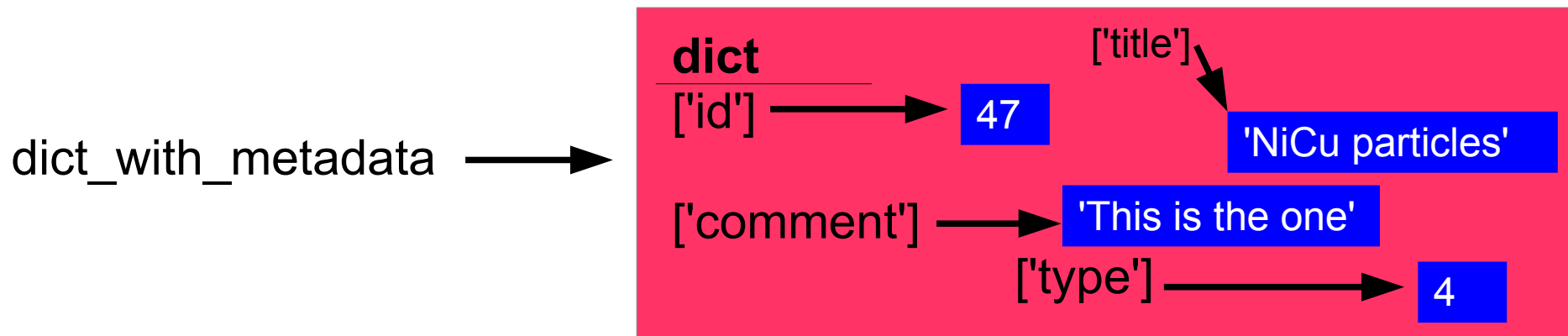


- Make a list with [] and with list() (e.g. by calling it in a string)
- Get objects out and save new values by index
- Try and write two integers as index separated by ':' e.g. mylist[1: 3]
- Make a list with two elements in and try:
`my_variable_a, my_variable_b = mylist`
- Try the index and count methods
- Exercises 9 and 11 on codecademy
- Call dir and help e.g. on a list and a string and read a little about some of the methods

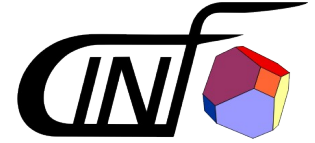
A mapping container – the **dict**



- Short for *dictionary*
- An **un-ordered mapping** of keys to values
- Objects are retrieved or assigned with keys
- Create a dict with {} or by calling dict() on a sequence of two-object sequences



Creating a dict



Start end end
curly parenthesis

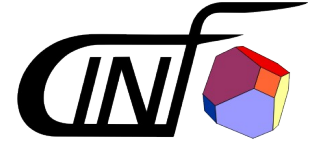
key, value **pair**

key value pairs
separated by ,

key and value
separated by :

```
>>> mydict = {key0: value0, key1: value1}
>>>
>>> dict([[key0, value0], [key0, value0]])
```

Index by keys



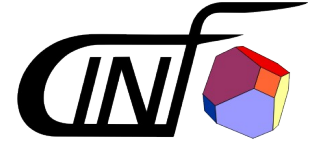
- Index a dict by **a key**
- Like look up word in a dictionary
- A key can be any object that cannot be changed

```
>>> mydict = {'title': 'CuZn', 0: True}
>>> mydict
{0: True, 'title': 'CuZn'}
>>> mydict[0]
True
>>> mydict['title']
'CuZn'
```

Index with square
parenthesis like list

The key

Also assign by key



- To assign a new value to an existing key, use: **[key]**

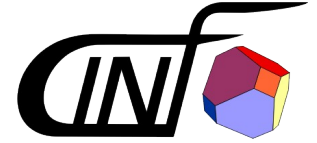
```
>>> mydict
{0: True, 'title': 'CuZn'}
>>>
>>> mydict['title'] = 'CuZn nano particles'
>>>
>>> mydict
{0: True, 'title': 'CuZn nano particles'}
>>> mydict['title']
'CuZn nano particles'
```


Dicts has lots of useful methods



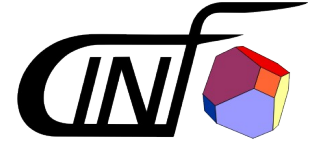
- **keys()** list of all the keys
- **values()** list of all the values
- **items()** list of all the key-value pairs
- **pop()** return value and remove it
- **update()** update values with values from another dict
- **get()** is like `[]` but does not give an error if the key is not in the dict
- ... and many more ...

Dict – Type along

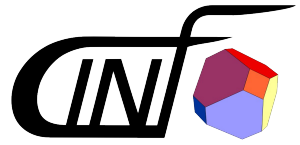


Type along session in the terminal:
Dict

Dict - Exercises



- Make a dict by entering it with `{}`
 - Try and use different types as keys and values
- Get objects out by indexing
- Assign a new value to one of the keys
- Try the *keys*, *values* and *items* methods
- Make a new dict that share some keys and has a few new ones compared to the first one and try and use the *update*
- Try *len()* on a dict
- Call *dir* and *help* on a dict and read a litte about some of the methods

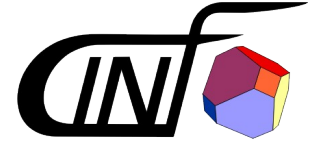


Center for Individual Nanoparticle Functionality

- What is a computer program
- Math
- Types
- Variables
- Containers
- Loops
- Boolean expressions
- Control flow (if-elif-else)
- Functions

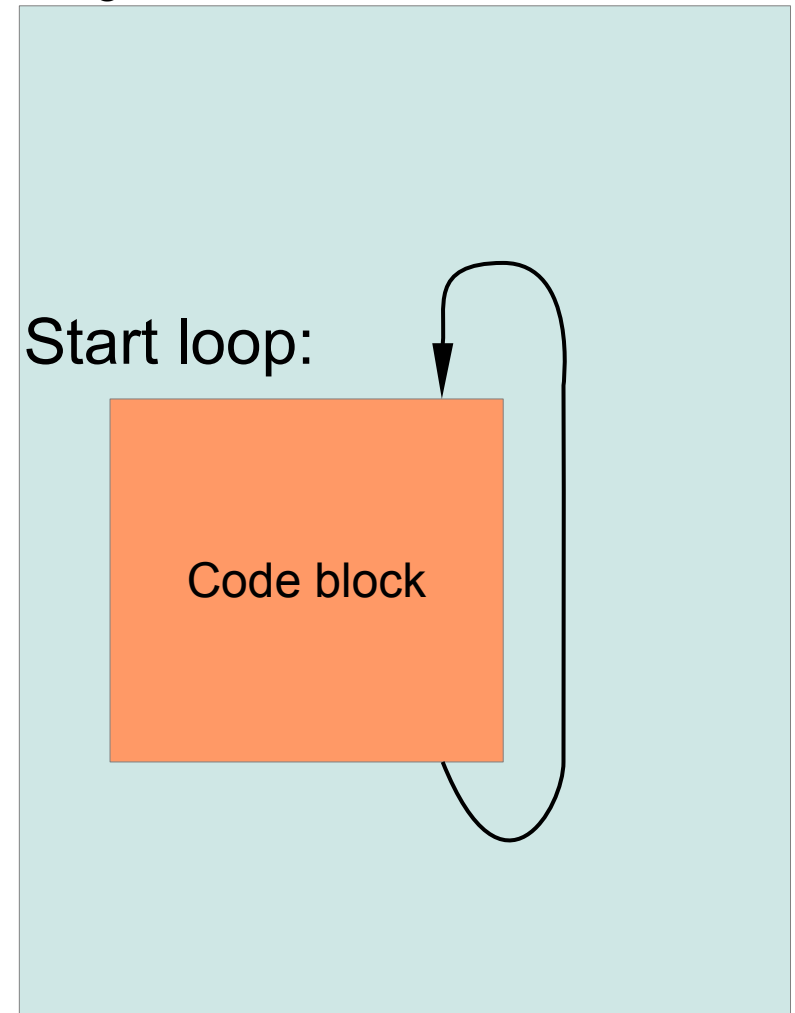
Python part 0

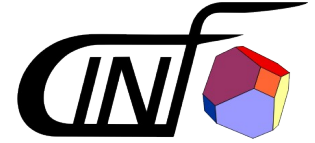
Loops



- Loops are fundamental to programming
- Repeat a part of program with different input
- E.g. once for every data set
- Python makes it easier

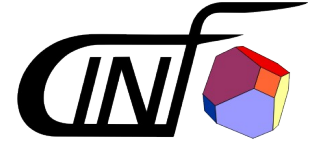
Program





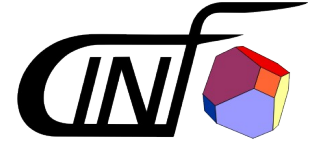
- The **for** loop
- Execute the block once for every object in sequence
- And make that object available in code block
- Used whenever you want to do the same thing for a sequence of somethings
- Think: *foreach measurement in my set, analyse and plot*

Loops **for** - example



```
>>> colors = ['magenta', 'cyan', 'crimson']  
>>> for color in colors:  
...     print color  
...  
magenta  
cyan  
crimson
```

Loops **for** - example



The “placeholder” variable name, the the object in the sequence will be assigned one after another

The sequence

```
>>> colors = ['magenta', 'cyan', 'crimson']
>>> for color in colors:
...     print color
...
magenta
cyan
crimson
```

The prompt changes to ... to indicate a block of code

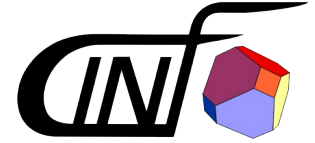
The result

The block of code

Notice the : that indicates that a block of code is about to start

The spaces indicate a block

About **code blocks**



- Indicates a “group on lines of code”
- That belongs to the line just before
- Sometimes done with parenthesis – in Python we use indentation

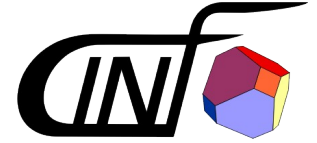
The : indicates the beginning of a block

```
for color in colors:  
    ...mystr = color + “ yeah”  
    ...print mystr
```

That block will continue as long as the lines are indented

Use 4 spaces for indentation. Your editor will help you, just press tab

Loops – Type along

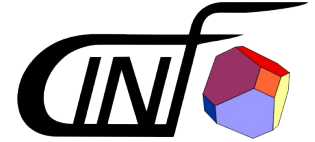


Type along session in the terminal:
Loops



- The **while** loop
- Execute the block for as long as an expression evaluates as True
- Used e.g. when one needs to check if something is complete
- Think “*keep doing this as long as ...*”

Loops – while example



```
counter = 3
while counter > 0:
    print counter
    counter = counter - 1
print 'Boom!'
```

Check, execute (again) if True

Block

Output

3

2

1

Boom!

Loops – while, more examples



- Empty a container

```
>>> colors = ['magenta', 'cyan', 'crimson']
>>> while len(colors) > 0:
...     print colors.pop()
...
crimson
cyan
magenta

>>> colors
[]
```

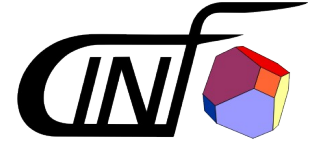
Loops – while, more examples



- Loop forever

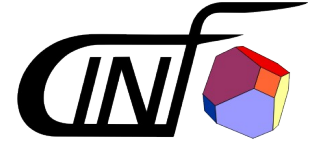
```
>>> while True:
...     # Keep doing this until the end of time
...     print "I am still here"
...
I am still here
I am still here
I am still here
I am still here
I am still here
```

About comments



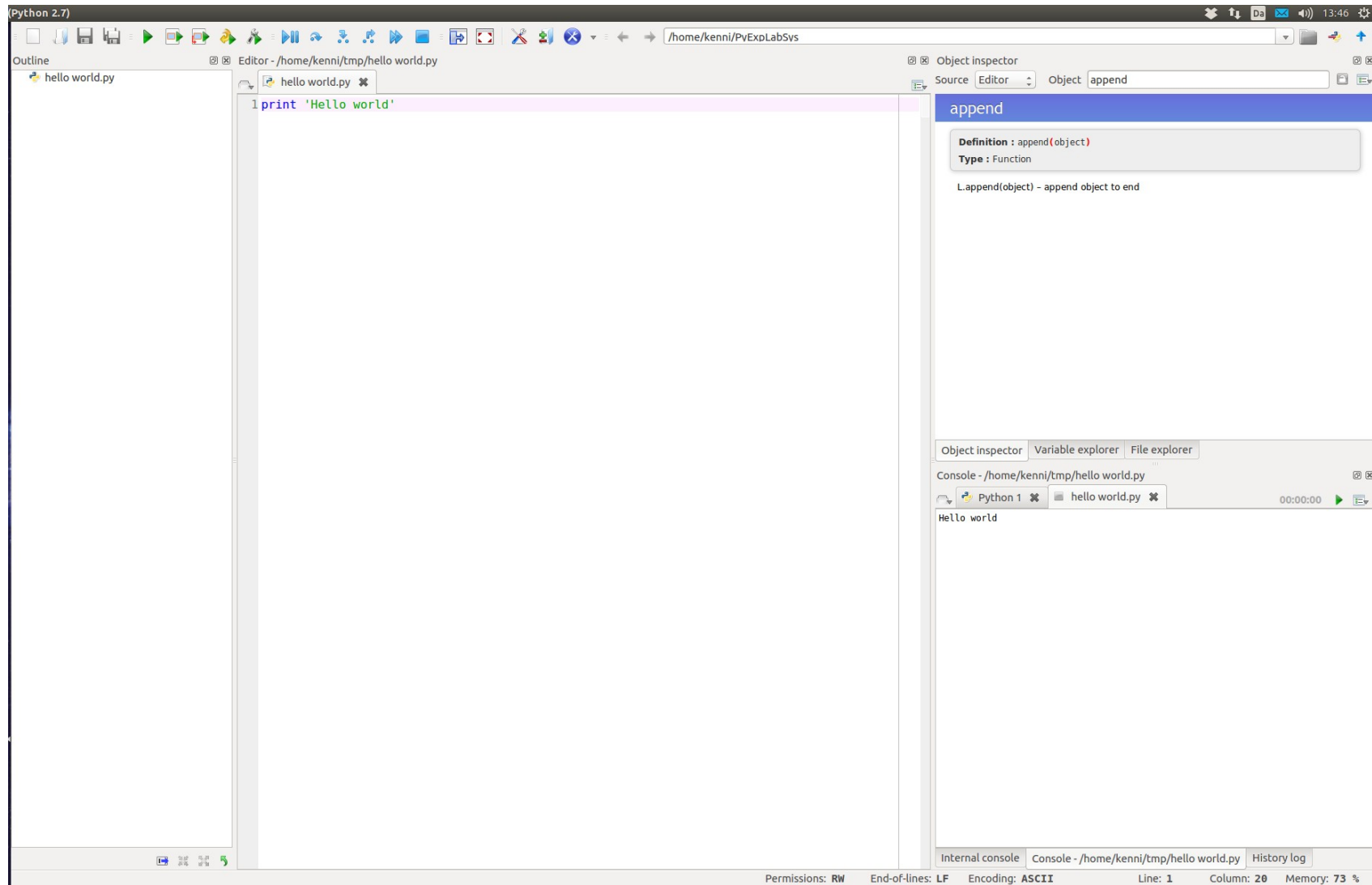
- Comments are lines of code that are not executed
- Used to explain the program to yourself
- A comment is made by starting a line with #

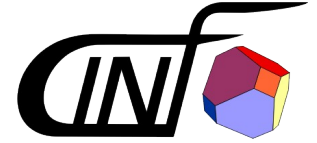
```
# Perform super fancy calculation  
result = 2 + 2
```



- The interpreter is really good for trying things out, but we do not want to keep typing the same things over and over again
- Python code can also be executed from a file
- We will write these files with an text editor called “Spyder”

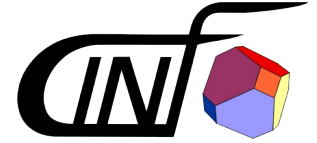
Spyder





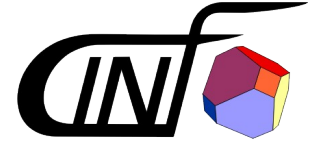
All type along sessions and exercises from now
on are in Spyder

Loops – Type along



Type along session in the terminal:
Loops

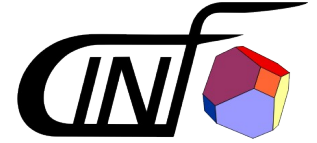
Loops – Exercises **IMPORTANT!!!**



- Make a list of strings and make a new list, by looping over the old, modify the strings and append it to the new list
- Make a variable with the value 1. Make a while loop that keeps multiplying it with 0.5 until the result is below $1\text{E}-8$. Print out the result: `7.450580596923828e-09`
- Work through problems 12-19 on codecademy

“Loop like a native”

<https://www.youtube.com/watch?v=EnSu9hHGq5o>



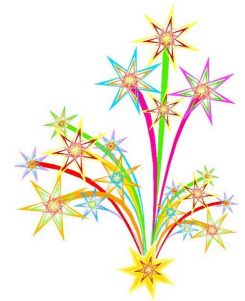
- In Python we **never ever** use integer indices to access object in a sequence (except arrays)
- Because it is error prone (of by one errors)
- People behind Python has taken care you do not need to

```
for color in colors:  
    print color
```

range(5) returns [0, 1, 2, 3, 4]

```
for index in range(len(colors)):  
    print colors[index]
```

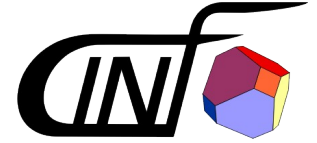
YES



NO!!!

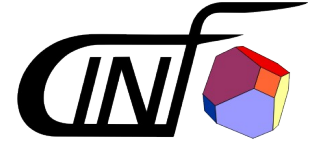


for loops the good way



- What if I need the index?
- Get the index along with the object
enumerate()
- What if I have more than one sequence?
- Loop over several sequences at once
zip()

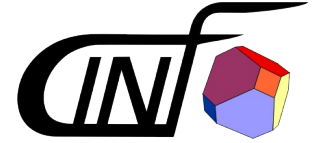
Remember unpacking?



- Assign several value from a list to multiple variables at once

```
>>> mylist = [47, -1]
>>> value1, value2 = mylist
>>> value1
47
>>> value2
-1
```

enumerate – enumerate objects

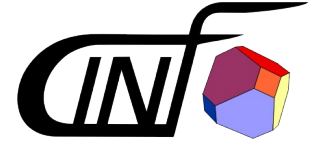


- Returns index-object pairs
- Can only be used directly in for loops
 - For use else-where call list on it: `list(enumerate(...))`

Notice un-packing in a for loop

```
>>> for index, color in enumerate(colors):  
...     print 'Color ' + str(index) + ' is ' + color  
...  
Color 0 is magenta  
Color 1 is cyan
```

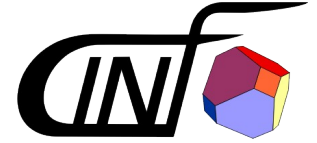

zip – pair objects in sequences



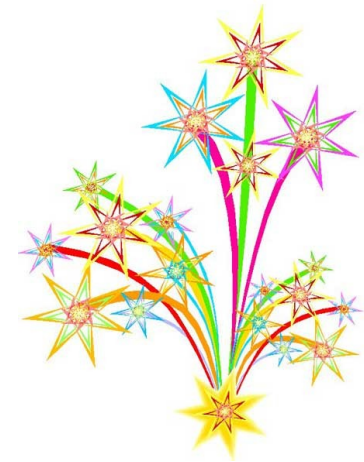
- Turns a pair of sequences into a sequence of pairs
- Can also only be used directly in for loops

```
>>> colors = ['magenta', 'cyan', 'crimson']
>>> shapes = ['square', 'circle', 'triangle']
>>> for color, shape in zip(colors, shapes):
...     print color, shape
...
magenta square
cyan circle
crimson triangle
```

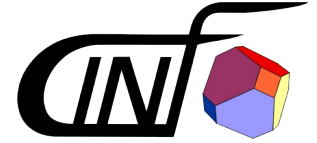
You are now a native



- Congratulations, you are now a Python native
- That is 90% of what you need to know, to *loop like a native*
- Enjoy!

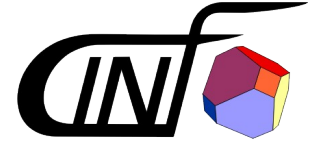


Loop like a native – Type along

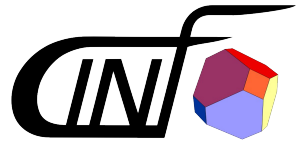


Type along session in the terminal:
Loop like a native

Loop like a native – Exercises **IMPORTANT!!!**



- Make a list of measurement descriptions e.g: ['C1s', 'O1s']
- Make a list of measurement ids e.g: [47, 147]
- Loop over both the lists and print a plot legend out by concatenating them e.g: 'C1s – 47'
- Instead of printing them, add them to a new list of legends
- Using enumerate and this new list, print out a new set of legends in which they are enumerated e.g: 'Plot 0: C1s – 47'
- Experiment with using three lists in zip
- Experiment with using 2 lists in zip, but where they do not have the same length. What happens?



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Python part 0

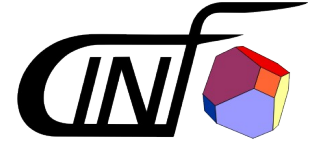
Boolean expression



- An expression that evaluates to True or False
- Used to make checks and perform decisions
- Simple (binary) operators are:

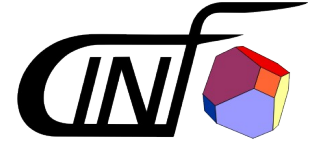
Operator	Explanation	Example	Result
>	greater than	5 > 5	False
>=	greater than or equal	5 >= 5	True
<	smaller than	-3 < 10	True
<=	smaller than or equal	47 <= 1	False
==	equals (carefull with floats)	10 == 10	True
!=	not equals	10 != 10	False
in	in (a sequence)	4 in [1, 2, 4, 7]	True

Boolean expressions



```
>>> 4 < 5
True
>>>
>>> 5 != 10
True
>>> 5 != 10
True
>>>
>>> 7 in [1, 2, 3]
False
>>> 3 in [1, 2, 3]
True
```

Special operator **not**



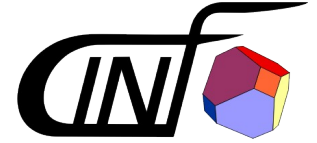
- **not** is a single argument operator that negates the following expression
- Special syntax for **in** (and is) for readability
- Also works with **!=**

Works on the argument after
(the result of $4 < 5$)

Works on the arguments
before and after (4 and 5)

```
>>> not 4 < 5  
False
```


not



```
>>> 4 < 5
```

```
True
```

```
>>> not 4 < 5
```

```
False
```

```
>>> 4 in [2, 4, 6]
```

```
True
```

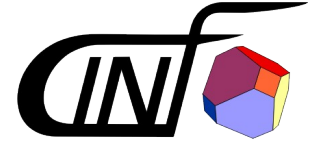
```
>>> not 4 in [2, 4, 6]
```

```
False
```

```
>>> 4 not in [2, 4, 6] # Also works
```

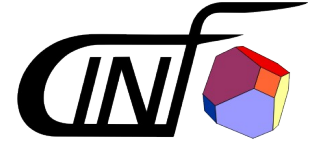
```
False
```

Putting boolean expression together



- Boolean expression can be put together to create more complex expressions for checks or decisions
- Binary operators **and** and **or**
- **and** - True when both are True
- **or** – True when at least one is True

Truth tables



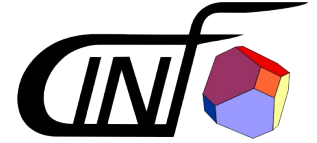
and

A	B	Result
True	True	True
True	False	False
False	True	False
False	False	False

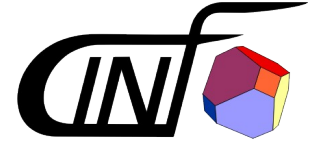
or

A	B	Result
True	True	True
True	False	True
False	True	True
False	False	False

Putting boolean expressions together



```
>>> 4 < 5 and 1 < 2
True
>>> 4 < 5 and 1 > 2
False
>>> 4 < 5 and not 1 > 2
True
>>> 4 < 5 and 2 in [2, 3]
True
```

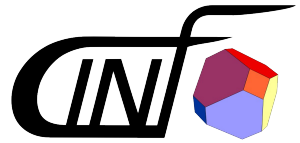


Type along session in the terminal:
Boolean expressions

Boolean expressions – Exercises



- Make an expression that checks if a number is in range i.e. between two others
- Make two sets of metadata in a dict e.g:
`{'label': 'C1s', 'monochromator': True}`
`{'label': 'O1s', 'monochromator': False}`
- While testing on both
 - Make an expression that checks whether it is a C1s measurement
 - Make an expression that checks whether it is monochromated
 - Make an expression that checks for both conditions
 - Make an expression that checks for either
 - Make an expression that check fo C1s and NOT monochromated



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Python part 0

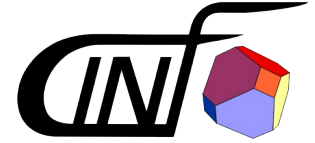
Control flow (if-elif-else)



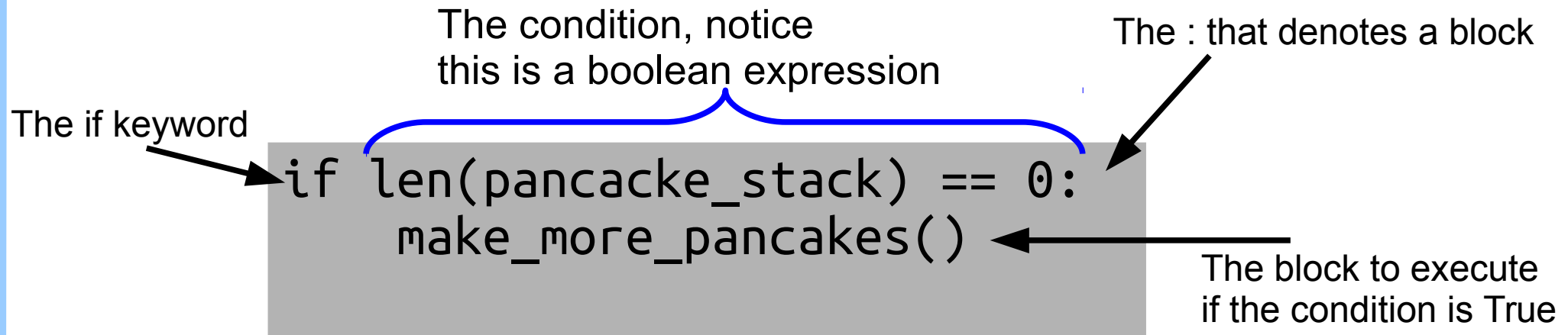
- Used to make decisions
- Code is executed from the top down
- A decision represents a cross-roads
- Execute only certain lines of code depending on a boolean expression
 - Aha! That is what they are for
- Decisions are very fundamental to all programming



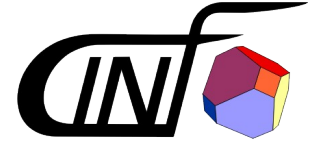
The **if** statement



- The simple **if** statement is used to optionally execute something
- Think “If these conditions are met, also do this”
- “If pan-cake plate is empty, make more”



The **if-else** structure



- Do something if and in all other cases do something else
- Think “If this is the case, do this, and if not, do something else”
- Classic cross-roads
- Always execute one block or the other

```
if len(pancacke_stack) == 0:  
    make_more_pancakes()  
else:  
    keep_eating()
```

Notice: No condition
after an else statement

The else block

The **if-elif-elif-else** structure



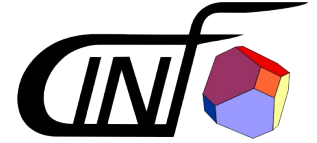
- **elif** is short for “else if”
- Adds the option, to one or more extra specific conditions to the decision, before the default **else**

```
if len(pancacke_stack) == 0:  
    make_more_pancakes()  
elif len(pancake_stack) == 1:  
    heat_up_pan()  
else:  
    keep_eating()
```

Note: The elif also has an condition

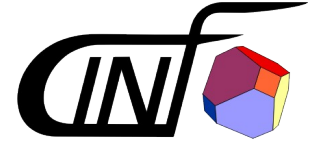
The **elif** block

The complete **if-elif-else** structure



- Note, the else is optional, also after elif
- The complete allowed structure is:
 - 1 **if**
 - Followed by 0 or more **elif**
 - Followed by 0 or 1 **else**

if-elif-else – Type along

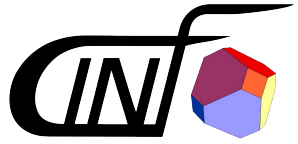


Type along session in the terminal:
if-elif-else

if-elif-else – Exercises



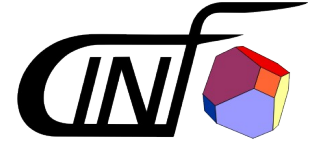
- Make a structure that checks a number and optionally prints out a message if the number is <0
- Make a structure that checks if there is content in a list and prints out two different message is there is and if there is not
- Make a structure that cheks an age, <13 (child), >65 (senior) and in between (adult) and prints out an appropriate greeting for each age group
- Make a structure that checks if a number is in range, is it if prints out the number and if not prints out a warning



Center for Individual Nanoparticle Functionality

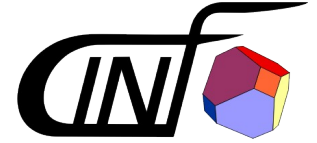
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Python part 0



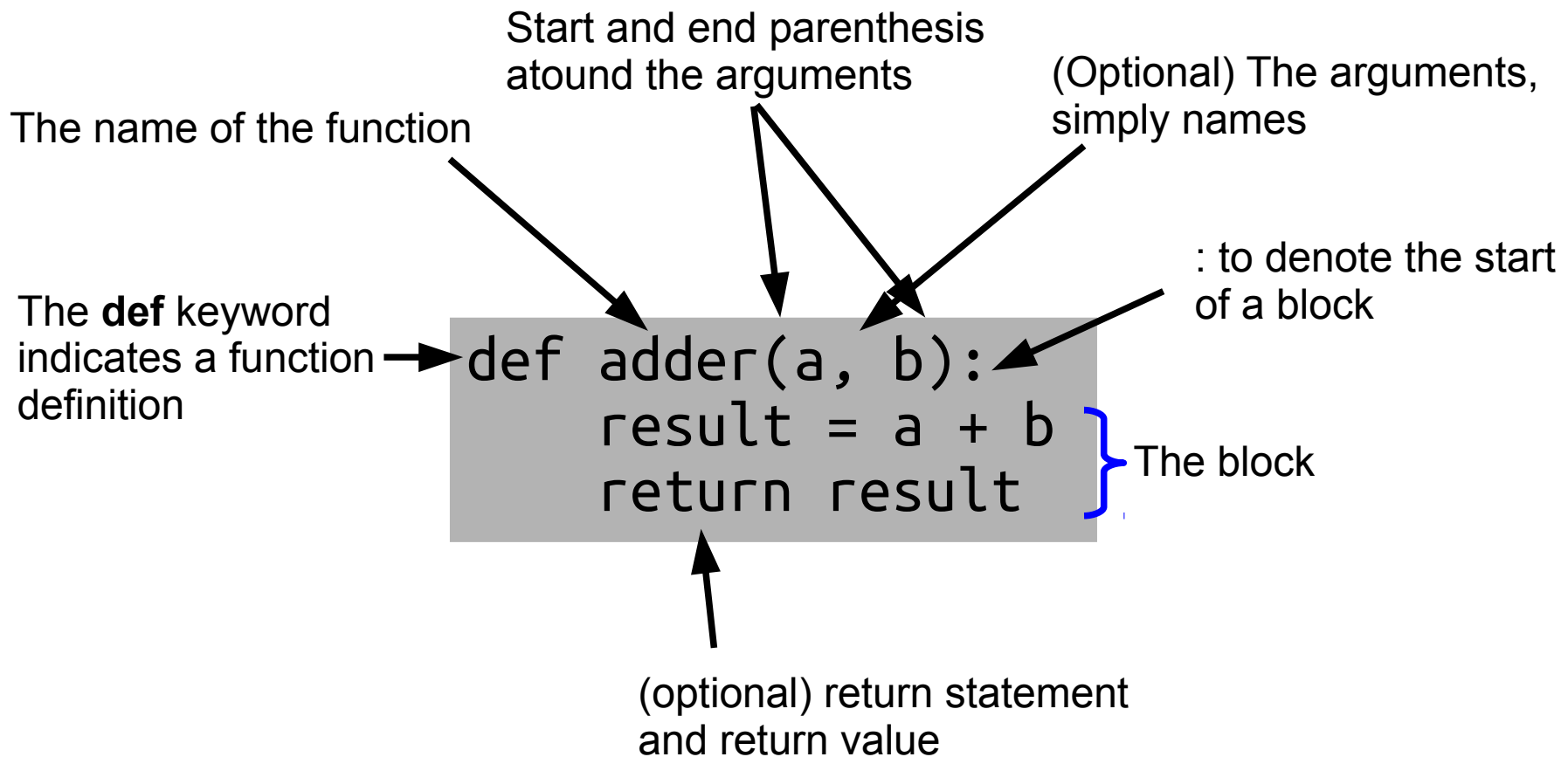
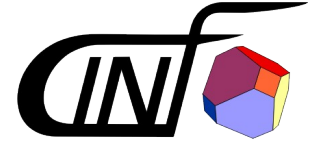
- A group of lines with well-defined (optional) input and (optional) output
- Used to:
 - **Re-use certain pieces of code**
 - **Organisation, to break up code into logical parts**
- *Very fundamental* to the way programs are structured
- Think “Functions perform a well defined job”
- This is where programming starts to get practical

The anatomy of a function



```
def adder(a, b):  
    result = a + b  
    return result
```

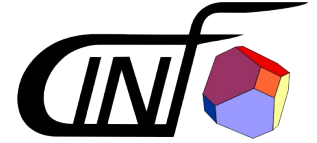
The anatomy of a function



More on functions



- Variables defined inside functions, including arguments, exist only inside the function
- The arguments are optional, but the () are not
- The return statement is optional, if missing the function will return None
 - Remember **None** means “nothing to see here”



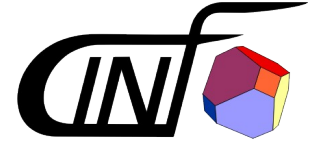
- Arguments are used in order

```
def adder(a, b):  
    result = a + b  
    return result
```

```
adder(1, 2)
```

```
# a will be 1 and b will be 2
```

Function examples



- Perform task, no return

```
def print_metadata(metadata):  
    print 'Title: ' + metadata['title']  
    print 'Id: ' + str(metadata['id'])  
    print 'Comment: ' + metadata['comment']  
  
my_meta = {'title': 'C1s', 'id': 47, 'comment': 'This is the one'}  
  
print_metadata(my_meta)
```

Function examples

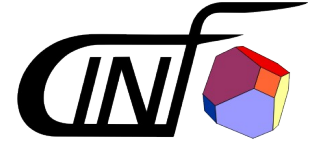


- Perform task, with return

```
def make_metadata_string(metadata):  
    result = 'Title: "' + metadata['title']  
    result = result + '" Id: ' + str(metadata['id'])  
    result = result + ' Comment: "' + metadata['comment'] + '"'  
    return result  
  
my_meta = {'title': 'C1s', 'id': 47, 'comment': 'This is the one'}  
  
metadata_string = make_metadata_string(my_meta)  
print metadata_string  
  
# Output  
Title: "C1s" Id: 47 Comment: "This is the one"
```

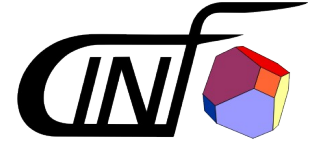
There is a better way to format numbers into strings, we will talk about that in part1

Function can call other functions



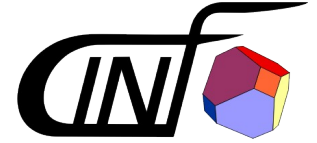
- Function can call other functions
- This is the way you make structure when complexity of you task increases
- They can also call themselves (recursion), but be carefull, that can produce infinite loops

Function can call other functions

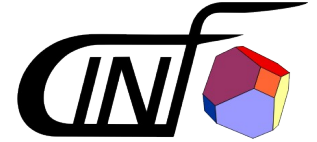


```
def perform_subtask0():  
    print 'Hello'  
  
def perform_subtask1():  
    print 'world'  
  
def perform_task():  
    perform_subtask0()  
    perform_subtask1()  
  
perform_task()
```


functions – Type along



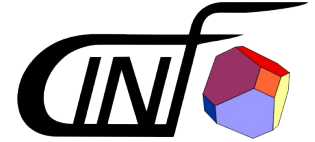
Type along session in the terminal:
functions



- Write a function “calculate” that performs a calculation with several parameters and call it
- Write a function “do_calculate” that calls the “calculate” and call it
- Write a function that returns the sum of every other element in a list
- Write a function that, given a list, returns a new list where all objects are multiplied by 2

Putting it all together

Putting it all together



```
# ... get_data and get_normalization not show

def analyze_data_set(data_set, normalization):
    # Fancy analysis
    return result

def analyze_data_sets(data_sets):
    normalization = get_normalization(data_sets)
    results = []
    for data_set in data_sets:
        result = analyze_data_set(data_set, normalization)
        results.append(result)
    return results

def main():
    data_sets = get_data()
    results = analyze_data_sets(data_sets)
    # plot data sets and results

main()
```



Center for Individual Nanoparticle Functionality

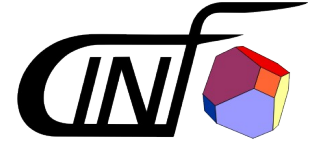
- Summary

Python part 0

Scientists Summary



- Math: Take care with division
- Objects have a type that defines what they can do
- Variables are names for objects
- Lists and dicts are the bread and butter of containers
- Use for and while loops for repetition
 - And loop like a native
- Boolean expressions, put together **and**, **or**
- If-elif-else to make decisions
- Functions for calculation, organisation and code re-use



- Getting good at a new syntax (e.g. Python) has a lot to do with muscle memory

Start writing Python and do it today

- Work through this tutorial:

https://openhatch.org/wiki/Boston_Python_Workshop_8/Friday/Tutorial

(and do actually type all the examples), for the repetition and for getting to type some more

- The link above is also to a large part the inspiration to this presentation

More optional homework



- <http://codingbat.com/python>

Elementary exercise that you can run on the website. Good for that muscle memory.

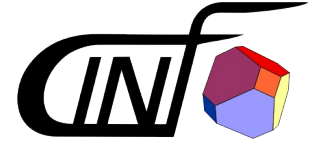
- <http://learnpythonthehardway.org/book/>

(Don't mind the comments about using a specific environment)

Have fun and see you at part 1

THE END

Extra slides, won't need them



- `abs()`
- `min()`
- `max()`
- `bool()`
- `any()`
- `all()`
- `is`
- `id()`
- `sum()`
- `round()`