

Lab 02 – Mini-Lecture

Scripting with Bash and Python

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NERS/ENGR 570 - Methods and Practice of Scientific Computing (F20)

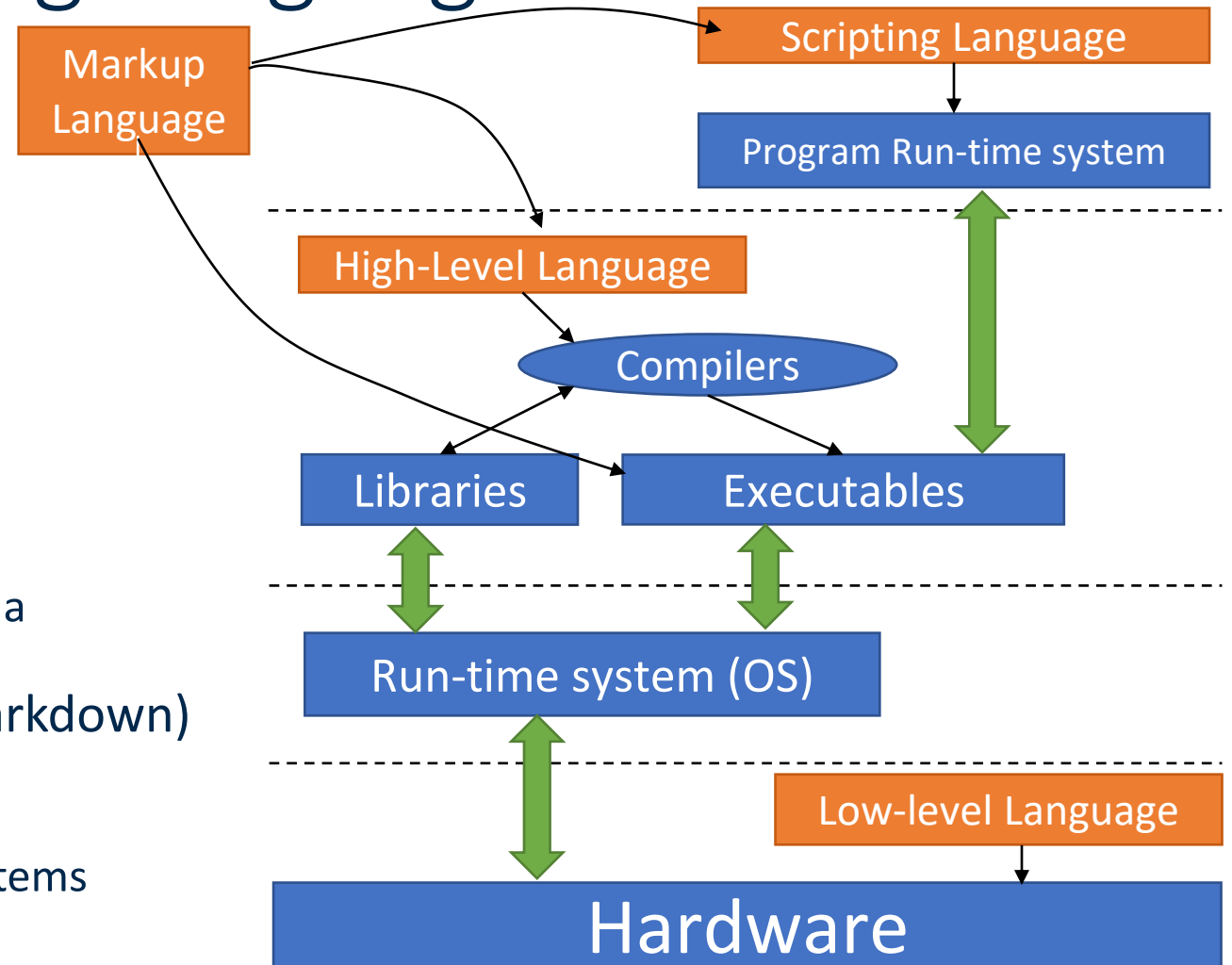


Outline

- Introduction to Bash Scripting (in 10 minutes)
- Introduction to Python (in 10 minutes)

Types of Programming Languages

- Low Level language (Assembly)
 - Defined by hardware (less portable)
- High Level language (C/C++, Fortran, Java)
 - Defined by run-time system (e.g. Operating System)
 - Portable, depends on compilers
- Scripting language (MATLAB, Python, Bash)
 - Defined by portable run-time system of a program
- Markup language (e.g. XML, YAML, Markdown)
 - Used for annotation
 - Data transfer
 - Input to multiple types of programs/systems



Shell Scripts in Linux

- Scripts are just text files
- First line is special

Bash Hello World

```
#!/bin/bash  
echo "Hello World!"
```

Python Hello World

```
#!/usr/bin/python  
print("Hello World!")
```

Perl Hello World

```
#!/usr/bin/perl  
print("Hello World!\n");
```

Awk Hello World

```
#!/usr/bin/awk -f  
BEGIN {  
    print "Hello World!"  
}
```

Symbol is sometimes called “bang”

Symbol is sometimes called “sha”

Program for interpreting the script

Together it is called
“Shebang”

```
#!/usr/bin/python  
print("Hello World!")
```



Scripting with Bash

More documentation at Too Long Didn't Program (tldp)

<http://tldp.org/LDP/abs/html/index.html>

Bash: The Basics

- The contents of your bash file will also work if entered correctly on the command line*

```
#!/bin/bash

# A comment

#print something
echo "Hello World"

#set a variable
myvar=1

#access a variable
echo $myvar
```

```
#!/bin/bash

# For loop
for i in 1 2 3 4; do
    echo $i
done
```

```
#!/bin/bash

# if else
touch newfile
if [ -e newfile ]; then
    echo "Found newfile"
else
    echo "Did not find newfile"
fi
```

*The exception here is script variables.

Pitfalls

```
#!/bin/bash

# A comment

#print something
echo "Hello World"

#set a variable
myvar=1

#access a variable
echo $myvar
echo "$myvar"
echo '$myvar'
```

No whitespace around
assignment operator!

Single quote
and double quote matter!

Variables defined in script do not persist after script!

Must have whitespace!

Test command "[" is
very confusing

```
#!/bin/bash

# if else
touch newfile
if [ -e newfile ]; then
    echo "Found newfile"
else
    echo "Did not find newfile"
fi
```

```
$ var=''
$ [ $var = '' ] && echo True
-bash: [: =: unary operator expected
$ [ "$var" = '' ] && echo True
True
$ [[ $var = '' ]] && echo True
True
```

Summary advice on Bash Scripts

When to use

- Simplifying complex commands
- Modifying files and directories
- Simple parsing and modification of file contents
- Working with operating system
- Generating inputs and jobs for parametric studies
- Some software project infrastructure tasks

When not to use

- Arithmetic
 - Especially floating point
- Data processing
 - e.g. parsing CSV files, finding max values, min values, averages
- Graphics (should be obvious)



Introduction to Python

It is the number 1 used programming language!

It is FREE!

It can do most anything other languages can do.

It is comparatively easier to use than high level languages.

There's a package for just about everything!

Executing python

- Interactively
 - Start a python “shell”: `$ python`
 - To exit the python “shell” enter: `Ctrl+d`
- Run a script
 - `$ python myscript.py`
- Run a script interactively
 - `$ python -i myscript.py`

Basic Syntax and Operators

Arithmetic Operators

```
print('Hello world')

x = 10.

print(x + 5.)
print(x - 4.)
print(x * 2.)
print(x / 3.)

print(x ** 2.)
# (x^2 in MATLAB)
```

Boolean Operators

```
x = 10.
# comparison
print(x == 15.)
print(x <= 12.)
print(x != 5.)

# boolean logic
print(not True)
print(True and False)
print(True or False)
```

Intrinsic types

- Python uses “dynamic typing”
 - No need to explicitly declare `int`, `float`, `bool`, etc.
 - Types are implied

```
x = 10.          #implied float
i = 1            #implied int
l = True         #implied bool
c = "Hello World" #implied string
```

- Declare variables anywhere!

#Python 2

```
2/3 == 0
2./3. == 0.66667
```

#Python 3

```
2/3 == 2./3. == 0.66667
2//3 == 0
```

Execution Control Constructs

If-Else

```
# indentation required:
if condition1:
    statements
elif condition2:
    other statements
elif condition3:
    other statements
else:
    alt statements
```

Looping

```
# i = 0, 1, ..., n-1
for i in range(n):
    print(i)

# iterate through a
# sequence
x_list = [1, 2, 4, 8]
for x in x_list:
    print(x)
```

Python Lists

- Effectively the implementation of arrays
 - Can be mixed “types”
- But these arrays are fancy
 - Can function like the classical data structure definitions of stacks, queues, or decks
- Operations on lists are very easy compared to other languages.
- Not very fast...
 - For speed you want numpy.

```
VY0 = [2., 3., 4.]  
print(VY0)  
print(VY0[0], VY0[-1])  
print(len(VY0))
```

```
VY0.append(5.)  
VY0[2] = "cat"  
print(VY0)
```

```
VY0.pop(0)  
print(VY0)
```

Further Reading

- Numpy and Scipy
 - <https://docs.scipy.org/doc/>
- Gorelick and Ozsvald, “High Performance Python,” O’Reilly Media, 2014.
 - <https://search.lib.umich.edu/catalog/record/018003128>
- MOOC: <https://www.sololearn.com/Course/Python/>
- A great new tool for productivity is the Jupyter Notebook
 - <https://jupyter-notebook-beginner-guide.readthedocs.io>