Welcome to Comp Sci 368-2!

Introduction to Scripting for CHTC

Overview, Course Mechanics, Introduction to Python

http://pages.cs.wisc.edu/~cs368-2/

Introductions

Instructor

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or (26)2-4002 *but email is best*

Background

- B.S., UW–Madison & Ph.D., John Hopkins (Cognitive Science)
- Software developer, educator, consultant
- ***Staff*** on CHTC team (not Professor)
- Open Science Grid (OSG) software and education

Course Objectives

Write basic code in Python

Solve scientific computing problems with scripting

Use Center for High Throughput Computing (CHTC)

Automate common scientific computing workflows

Syllabus

Python	1: Overview; Intro to Python
	2: Basic Syntax
	3: Collections
	4: I/O & Exceptions
	5: Data, Functions, and Classes
	6: Modules and the Standard Library
	7: Regular Expressions
	8: System Interaction
CHTC	9: Intro; Running Jobs
	10: More Complex Jobs
	11: Workflows with DAGMan
Scripting for CHTC	12: Scripted Workflows I
	13: Scripted Workflows II
	14: Wrapper Scripts
	15: Science Code in Python

Course Philosophy

Learn *a new skill*

Learn *by doing*

Learn *to fish*

My Suggestion:

Write code.
At least a little.
Every day.
Play around!

Course Mechanics

Credit and Homework

- **Credit**
  - Course offered as credit/no credit
  - All points come from homework (no exam)
- **Homework**
  - Short coding or CHTC assignment
  - Every day (except last day): 14 total
  - Due by 1:30 p.m. of next class (email tolerated)
  - ***No late assignments accepted at all***
  - Each homework given 0, 1, or 2 points
  - Need 18 points (64%) to get credit for the course

Homework Points

Pts	Reason
2	• turned in on time, AND • code runs, AND • solution is correct or nearly so, AND • demonstrates real effort
1	• turned in on time, AND • partial solution, may not actually run, AND • demonstrates some effort (my discretion)
0	• late, OR • ***is plagiarized (= Academic Misconduct)***, OR • does not demonstrate any real effort

Mailing List

compsci368-2-s12-hhh@lists.wisc.edu

- Goes to your **@wisc.edu** account
- Check spam filters
- Post questions, comments, and discoveries!
  - Except direct homework questions (see rules)
  - All else is fair game

Office Hours

Computer Sciences 4265 (Tim's office)

Days and times: Doodle poll today!

Other times available by appointment (email)

Python Resources

- Book: ***Learning Python*** (4th Ed.)
  - Available FREE online via MadCat
  - Not in the UBS textbook area
  - Note Python version info
- Python documentation
  `http://docs.python.org/release/2.4.3/`
- Python 2.4 Quick Reference
  `http://rgruet.free.fr/PQR24/PQR2.4.html`

Machines

- Computer Systems Lab (CSL) accounts
  - Old accounts may still be active
  - Otherwise, see login screen on instructional machines
  - Problems? Stop by CompSci 2350 (the CSL), or email **`lab@cs.wisc.edu`**
- Personal machine OK for Python, but check version
- Will get CHTC account later

Scripting in Python

Why Scripting?

- Abstracts over low-level details
- Rapid development
- Easy to understand and change
- Pervasive

Why Python?

- Powerful: Has everything you need
- Clear: Modern, clean design
- Highly portable: Runs nearly everywhere
- Widely used in scientific computing

Python vs. C++: Print a File

Python

```
inStream = open("Data.txt", "r")
for line in inStream:
    print line
```

C++

```
#include <iostream>
#include <fstream>
#include <string>
using namespace std;
int main() {
  ifstream InStream;
  string line;
  InStream.open("Data.txt");
  getline(InStream, line);
  while (! InStream.eof()) {
    cout << line << endl;
    getline(InStream, line);
  }
}
```

Python Versions

- ≤ **2.3** considered very old, not recommended
- **2.4** – **2.6** still very common
  - Red Hat Linux 5 has 2.4.3 *(CHTC submit machine)*
  - Red Hat Linux 6 has 2.6.6 *(instructional machines)*
  - Debian 6 (“squeeze”) has 2.6.6
- **2.7** is current, but end-of-line for **2.x**
  - Mac OS X 10.7 (“Lion”) has 2.7.1
- **3.x** is the future — but is ***not*** backward compatible

`http://wiki.python.org/moin/Python2orPython3`

Running Python

Interactive Python

```
$ python
Python 2.4.3 (#1, Dec 11 2006, 11:39:03)
[GCC 4.1.1 20061130 (Red Hat 4.1.1-43)] on
linux2
Type "help", "copyright", "credits" or
"license" for more information.
>>>
```

- Great for trying things out
- Cannot save state
- ∴ Not great for reuse

Running Python Scripts

- **Linux / Unix**
  - `python filename.py`
  - `chmod 0755 filename.py`
    `./filename.py`
- **Mac OS X**
  - Use Terminal, same as above
- **Windows**
  - Available from main Python website
  - Not officially supported in the course

Python Bootcamp … Starts Now!

Numbers

integers	`42  -13  0  123456`
really long integers	`1234567890123456789L`
floating-point numbers	`-0.5  3.141  2.7182818`
exponential notation	`2.998E8  6.022e23  6.626e-34`
integers in octal (base 8)	`0177  0377`
integers in hex (base 16)	`0x3A  0Xff  0x12ab`
complex numbers	`3+4j  -3.5+2.0j  6J`

(Some) Operations on Numbers

group	`24 * (3 + 4)`

calculate	`abs(-24.33)`
	`min(3, 4, 1, …, 8)`
	`max(3, 4, 1, …, 8)`
	`round(1234.56)`
	`round(1234.5678, 2)`

negate	`-x`
exponentiate (power of)	`2 ** 8` `pow(2, 8)`

multiply & divide	`42 * 3.141`
	`5.0 / 2  or 5.0 // 2.0`
	`23 % 5`

add & subtract	`12 + 34` `2011 - 1970`

Strings

string (single or double quotes)

```
'Hello, "world"!'
"Hello, 'world'!"
```

really long strings

```
"""Really long strings
can span multiple lines,
etc.  Newlines are kept."""
```

escapes

```
'one line\nsecond line'
"tab\tseparated\tdata"
"has \"quotes\" inside"
```

raw string

```
r'C:\new\test.txt'
```

(Some) Operations on Strings

concatenate	`'Hello, ' + "world!\n"`	`'Hello, world!\n'`
repeat	`'-' * 15`	`'---------------'`
index	`"hello"[1]`	`'e'`
	`"hello"[-1]`	`'o'`
slice	`"hello"[1:4]`	`'ell'`
functions	`len('hello')`	`5`
	`'  hello \n'.strip()`	`'hello'`
	`'CrAzY'.lower()`	`'crazy'`
	`'Hello'.find('el')`	`1`
	`'hello'.endswith('lo')`	`True`
	`'123.0'.isdigit()`	`False`

String Formatting

```
"… %d … %f … %s …" % (42, 3.1, 'text')
```

integer	`'Count: %d' % (123)`	`'Count: 123'`
float	`'Mean: %f' % (6.23 / 17)`	`'Mean: 0.366471'`
string	`'Hello, %s!' % ("Tim")`	`'Hello, Tim!'`
% character	`'C = %f%%' % (5 / 2.0)`	`'C = 2.500000%'`
multiple	`'L: %f%s' % (2.6, 'm')`	`'L: 2.600000m'`
advanced	`'%6.2f' % (1.23456789)`	`'  1.23'`

See book or online resources for lots more!

Strings ≠ Integers ≠ Floats

```
>>> 1 + '1'
Traceback (most recent call last):
  File "<stdin>", line 1, in <module>
TypeError: unsupported operand type(s) for +:
'int' and 'str'
```

Convert to *integer*	`int('5')` `int(5.1234)`
Convert to *float*	`float('5')` `float(5)`
Convert to *string*	`str(5)` `str(5.1234)`

Wrap Up

Homework

- **Part 1**
  - Visit course website, find homework #1 in syllabus
  - Run script given there; ***print and turn in output***
- **Part 2**
  - Run interactive Python session
  - Play around with numbers and strings
  - ***Print and turn in*** interesting discoveries
  - See homework #1 for details
- **Part 3 (sort of)**
  - Complete the survey (if you have not done so already)

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