Numerical Methods in Materials Science and Engineering
First Day

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Welcome to MSE 350

- I am not Dr. Erdmann! He is **out** for the week.
- Watch the NASA launch (http://countdown.ksc.nasa.gov/shuttle/countdown/cdt/)
- Laptop use in class is encouraged! (for programming related . . . )
- There is no assumption of previous programming experience . . .
- Prereqs: Vector and Diff-Eq.
Today

- This presentation: http://u.arizona.edu/~mgoodman/
- Class site: http://www.u.arizona.edu/~erdmann/mse350/
- Plagiarism Video http://deanofstudents.arizona.edu/
- Class overview
- HW for Wednesday
Academic Integrity “video”

Just don’t do it!

Fwd: New Academic Integrity video to show students on the first day of classes

Hey,

I just got this. As directed below, please show the academic integrity video during the week I'm gone. Also please emphasize that if the students cheat, I will personally hunt them down and brutally murder them regardless of the university policy that likely prohibits this.

Thanks.

-RGE
What is Python?

Python is a general-purpose high-level programming language. Its design philosophy emphasizes code readability. Python claims to “[combine] remarkable power with very clear syntax”, and its standard library is large and comprehensive. Its use of indentation as block delimiters is unusual among popular programming languages.[wik, ]
Why Python?

- Modern
- Modular
- Concise
- Powerful
- Interactive
- Cross Platform
Why Python? – Modern

- First Release in 1991!
- Under heavy active development
- Used by a number of giants:
  - YouTube, Google, BitTorrent
  - Yahoo!, CERN, NASA, OLPC
- Most Linux/Unix
Why Python? – Modern

From xkcd.com[xkc, ]
Why Python? – Modern

Wow Development!

antigravity 0.1

A really simple module that allow everyone to do “import antigravity”

File                     Type       Py Version       Uploaded on
antigravity-0.1.zip (md5) Source           |            2007-12-06 11:

Author: Fabien Schwob <antigravity at x-phutre com>
Home Page: http://fabien.schwob.org/antigravity/
Package Index Owner: fabienschwob
DOAP record: antigravity-0.1.xml
Why Python? – Modular

Some standard modules:

- os – Dealing with the operating system and files
- wave – Working with sound files
- gzip, tarfile, zipfile – Working with compressed files
- urllib, webbrowser – Retrieving web pages and interacting with the local web browser
- sqlite, tables, csv – Specialized database and data file formats.
- email, pidgin – Interface to email and chat clients.
Why Python? – Modular

Unique problems in programming are RARE.

▶ Reinventing the wheel == bad!
▶ Python modules offer engineered solutions to common tasks.
▶ This class will focus on several modules well suited to engineering and science related endeavors:
  ▶ Numpy – Powerful array operations
  ▶ Scipy – Scientific libraries
  ▶ MatPlotLib – Plotting http://matplotlib.sourceforge.net/gallery.html
  ▶ Mayavi – 3d visualization (demo) https://svn.enthought.com/enthought/wiki/Mayavi/Gallery
Why Python? – Modular

Modularity extends even to OTHER PROGRAMMING LANGUAGES

- SWIG – Generates python interfaces to many languages (Java, C, C++, FORTRAN, Perl . . . )
- Cython – Creates C code out of Python
- PyCUDA – Interface to the NVIDIA CUDA GPU computing platform
Why Python? – Concise

- Python was designed with readability in mind.
- Code is broken up with white-space
- More on this all later!

```python
print "hello world"
lunch_options = "spam, eggs, and spam"
if "spam" in lunch_options: print "Yay spam!"
```
Why Python? – Powerful

All of the following things could be **comfortably** accomplished in less than 10 lines of code thanks to the wealth of modules available:

- Monitor an industrial process and send an email in case of disruption.
- Connect to a remote database and perform a complex query and display/save the results.
- Take the symbolic integral of a complex function.
- Visualize a 2d or 3d data set with interactive display
- Download a large number of files from a website on an automatic schedule.
- Load an image, perform several filters and save it as a different format.
- Write an alarm clock with user specified wait time and music ramping.
- Make a chat-robot that harasses your friends.
Why Python? – Interactive

Demo time!

- Interactive help
- Interactive programming
- Interactive HPC
Why Python? – Cross Platform

- Supports all major operating systems
  - Linux
  - Windows (95, XP, Vista, 7?)
  - Mac OSX
- Portable code!
HW1: Get Python

Downloading and Installing the following is your homework for the next class:

- python – the Python interpreter
- ipython – the interactive Python interpreter
- A text editor – 100+ options here ...
HW1: Continued . . .

Also, we will need the following modules:

- numpy
- scipy
- matplotlib
- tables
- mayavi
You could track down all these individual installs and files, but it is much easier to download a bulk distribution that includes all of these tools:

- The Enthought Python Distribution (EPD) found at [http://www.enthought.com/](http://www.enthought.com/). (all platforms)
- python(x,y) the “full” distribution found at [http://www.pythonxy.com/](http://www.pythonxy.com/). (ia-64 not supported?)
- From the Linux apt repositories (ask me for a package list) (Debian/Ubuntu)
Completing HW1

The final three steps:

1. Download the python script found here (http://www.u.arizona.edu/~mgoodman/)
2. Run it
3. Send a screen shot of everything working well to me at mgoodman@email.arizona.edu
4. Please include your full name, and a “secret-name/moniker” under which grades will be posted (if you don’t choose one, I will and you probably won’t like it)
Working Configuration

This is good:

```
Terminal - meawoppl@meawoppl-mini: ~/erdmann-sub

File Edit View Terminal Go Help

/__init__.pyc'
Successfully loaded: <module 'scipy' from '/usr/lib/python2.6/dist-packages/scipy/__init__.pyc'>
Successfully loaded: <module 'matplotlib' from '/usr/local/lib/python2.6/dist-packages/matplotlib/__init__.pyc'>
Successfully loaded: <module 'enthought' (built-in)>
Test Successful!
Mail a screenshot of this to mgoodman@email.arizona.edu

meawoppl@meawoppl-mini:~/erdmann-sub$ python test all imports.py
Successfully loaded: <module 'numpy' from '/usr/lib/python2.6/dist-packages/numpy/__init__.pyc'>
Successfully loaded: <module 'scipy' from '/usr/lib/python2.6/dist-packages/scipy/__init__.pyc'>
Successfully loaded: <module 'matplotlib' from '/usr/local/lib/python2.6/dist-packages/matplotlib/__init__.pyc'>
Successfully loaded: <module 'enthought' (built-in)>
Test Successful!
Mail a screenshot of this to mgoodman@email.arizona.edu
Press any key to continue ...
```

meawoppl@meawoppl-mini:~/erdmann-sub$  

Lastly . . .

- If you have any trouble . . .
- Please also begin reading the first three sections of the python tutorial found at:
  - http://docs.python.org/tutorial/
- We will have covered all of that material by the end of Wednesday if all goes well.
Bibliography I

Wikipedia, the free encyclopedia.

Xkcd, a webcomic of romance, sarcasm, math, and language.