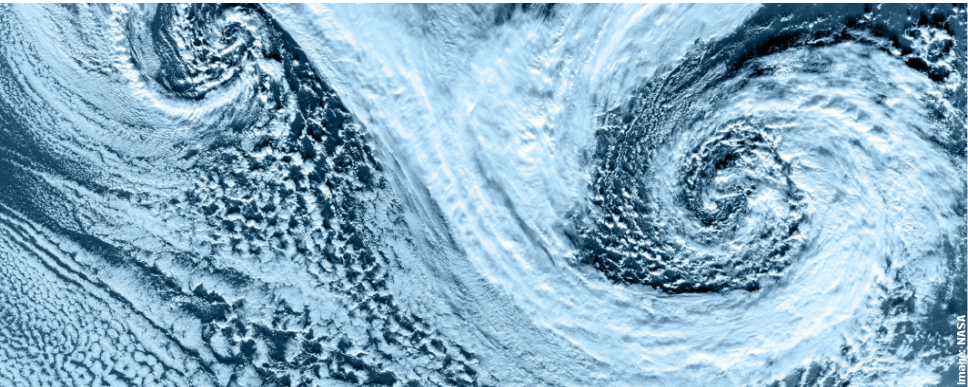


C2SM workshop

Scientific Programming in Python

Harald von Waldow (C2SM) Bas Crezee (IAC/Atm.Dyn.)
Nicolas Piaget (IAC/Atm.Dyn.) Marina Dütsch (IAC/Atm.Dyn.)

2014-09-11



Schedule

| | | |
|--------|---------------------------------------------------------------|-------------------|
| 09:30 | Welcome, organizational matters | Harald |
| 09:45 | Python — The big picture | Harald |
| 10:00 | Python development tools | Harald |
| 10:15 | Exercise 1: The IPython Notebook — First steps | Bas |
| 10:45 | Coffee Break 15 min | |
| 11:00 | Exercise 2: Syntax, Control-Flow, Datastructures | Harald |
| 12:00 | Lunch Break 1 h | |
| 13:00 | Exercise 3: Numpy, Scipy, Matplotlib, basemap, netcdf4 | Nicolas |
| 14:30 | Coffee Break 15 min | |
| 14:45 | Exercises 4 & 5: The Big Exercise | Harald Nicolas |
| 17:00 | Other packages, Outlook | Harald |
| 17:15 | Wrap up, Discussion, Questions, Feedback | Harald |
| 17:30? | End | |

Organizational Matters

Room

- Is not going to be locked during breaks.
- Take your valuables with you.
- Logout or lock screen

Organizational Matters

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IT-setup

- On your local desktop runs a browser.
- The browser connects to a local port (7777), which is forwarded to a port on our server.
- On that server runs the IPython-process, one for everybody, and all data resides there.
- That server is `iacdipl-3.ethz.ch`. You should not need to worry about that.

Organizational Matters

Login

- username: c2smXX
- XX is 02 ... 19
- password: -- censored --
- After login wait 10 sec or so ...
- In case of password-asking pop-up window: Click "cancel".
- the browser should start and load the proper page.

Python — the big picture

History, Versions

- A young and fast moving language by Guido van Rossum:
 - Python 1.0: 1994
 - Python 2.0: 2000
 - Python 2.7: 2010
 - Python 3.0: 2008
 - Python 3.4: 2014
- Python 3.x is incompatible with 2.x.
- New, large projects should be written in 3.x.
- For research code, often depending on exotic modules, use 2.7.
- Some new features can be made available in 2.7 using
`from __future__ import XY`

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Python — the big picture

Classification

- interpreted
- general-purpose, high-level
- dynamically typed
- garbage-collection
- multi-paradigm:
 - functional, object-oriented
 - procedural programming features

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Features

- **optimal for fast development**
- documentation well integrated with code
- clean, simple, intuitive
- expressive (= less lines of code)
- scales well with project size

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Python — the big picture

Advantages for scientific computing

- large and fast growing user community
- large and fast growing number of libraries for sci. com.
- well integrated with “bread-and-butter” codes, such as BLAS, LAPACK, Netlib standards such as ODEPACK, ...
- highly extensible, large collection of add-on packages
- easy communication with R, C, Fortran, ...

Python — the big picture

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Python — the big picture

When to use Python?

ALWAYS!

except:

- You need the speed of C or Fortran
- You can re-use significant code written in other languages.
- You do HPC (using MPI, OpenMP)
- You can profit from a non-Python tradition in your field or workgroup.
- Something else is better for the task, ...

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Other interpreted languages to consider

- R: lingua franca of statistics. There is no choice for advanced stats.
- You better know Python and R.
- Matlab: Some specialized toolboxes have (yet) no counterpart in Python.

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Python — the big picture

Philosophy

The Zen of Python (try “import this”)

- Beautiful is better than ugly.
- Simple is better than complex.
- Complex is better than complicated.
- Readability counts.
- There should be one— and preferably only one —obvious way to do it.
- ...

Python — the big picture

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Python programmers strive to write *pythonic*

- Don't get lost in beauty
- But if you have trouble understanding your own code ...
- ... after your holidays ...
- “import this” and re-factor a bit.

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The Zen of Python (try “import this”)

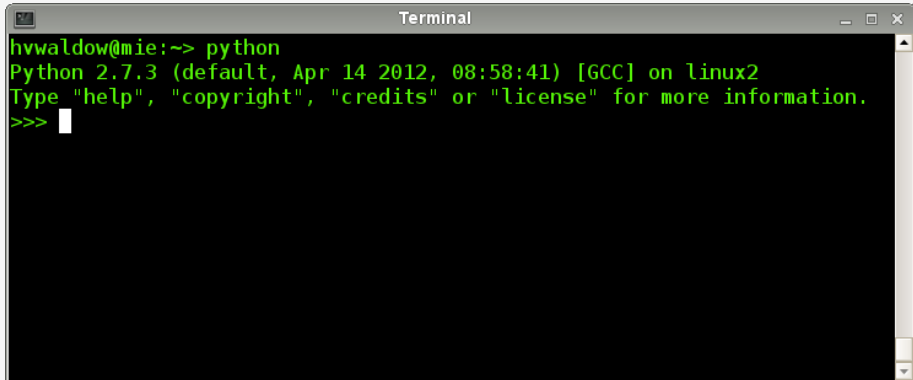
- Beautiful is better than ugly.
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Basic Python

Python shell

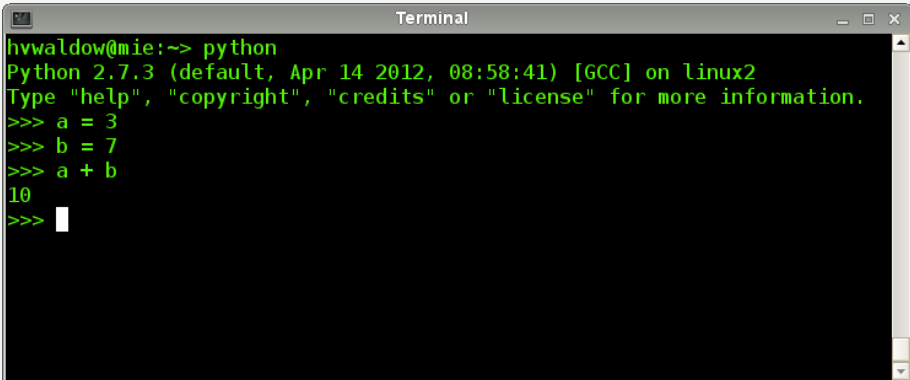
A terminal window titled "Terminal" with standard window controls. The text inside is green on a black background. It shows the command 'python' being executed, followed by the Python 2.7.3 startup banner and the prompt '>>>' with a cursor.

```
hvwaldow@mie:~> python
Python 2.7.3 (default, Apr 14 2012, 08:58:41) [GCC] on linux2
Type "help", "copyright", "credits" or "license" for more information.
>>> █
```

Typing “python” will call the “raw” Python shell.

Basic Python

Python shell

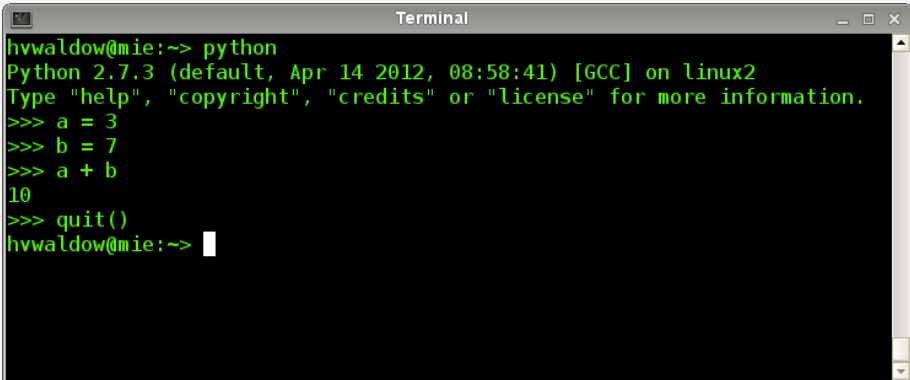
A terminal window titled "Terminal" with standard window controls. The prompt is "hvwaldow@mie:~>". The user enters "python", which starts the Python 2.7.3 interpreter. The interpreter displays its version and build information, then prompts for help. The user enters three lines of code: "a = 3", "b = 7", and "a + b". The interpreter outputs "10" for the last line. A cursor is visible on the line following the last input.

```
hvwaldow@mie:~> python
Python 2.7.3 (default, Apr 14 2012, 08:58:41) [GCC] on linux2
Type "help", "copyright", "credits" or "license" for more information.
>>> a = 3
>>> b = 7
>>> a + b
10
>>> 
```

Can be used like a calculator.

Basic Python

Python shell

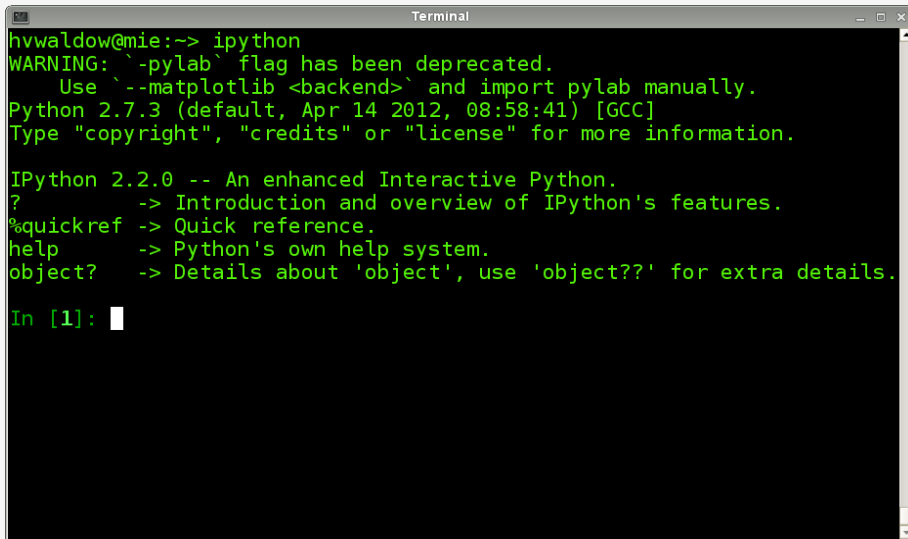
A terminal window titled "Terminal" with standard window controls (minimize, maximize, close) in the top right corner. The terminal shows a user at a prompt "hvwaldow@mie:~>" typing "python". The output shows "Python 2.7.3 (default, Apr 14 2012, 08:58:41) [GCC] on linux2" followed by a message to type "help", "copyright", "credits", or "license" for more information. The user then enters three lines of Python code: ">>> a = 3", ">>> b = 7", and ">>> a + b". The output of the last line is "10". Finally, the user enters ">>> quit()", and the prompt returns to "hvwaldow@mie:~>".

```
hvwaldow@mie:~> python
Python 2.7.3 (default, Apr 14 2012, 08:58:41) [GCC] on linux2
Type "help", "copyright", "credits" or "license" for more information.
>>> a = 3
>>> b = 7
>>> a + b
10
>>> quit()
hvwaldow@mie:~> 
```

Call function “quit()” to exit.

Basic Python

IPython shell

A terminal window titled "Terminal" with a standard macOS-style title bar (red, yellow, green buttons). The terminal has a black background with green text. It shows the command 'ipython' being executed at a prompt 'hvwaldow@mie:~>'. The output includes a deprecation warning for the '-pylab' flag, the Python version '2.7.3', and the IPython version '2.2.0'. It also lists several shortcuts: '?' for introduction, '%quickref' for quick reference, 'help' for Python's help system, and 'object?' for details about objects. The prompt 'In [1]:' is shown at the bottom with a white cursor.

```
hvwaldow@mie:~> ipython
WARNING: `-pylab` flag has been deprecated.
        Use `--matplotlib <backend>` and import pylab manually.
Python 2.7.3 (default, Apr 14 2012, 08:58:41) [GCC]
Type "copyright", "credits" or "license" for more information.

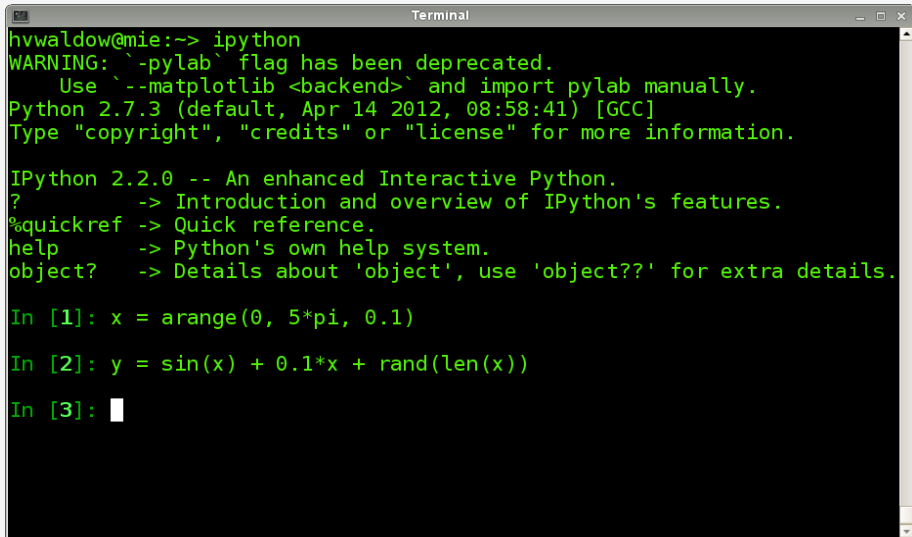
IPython 2.2.0 -- An enhanced Interactive Python.
?           -> Introduction and overview of IPython's features.
%quickref   -> Quick reference.
help        -> Python's own help system.
object?     -> Details about 'object', use 'object??' for extra details.

In [1]:
```

Typing “ipython” will call the IPython shell.

Basic Python

IPython shell



```
Terminal
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WARNING: `--pylab` flag has been deprecated.
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In [1]: x = arange(0, 5*pi, 0.1)

In [2]: y = sin(x) + 0.1*x + rand(len(x))

In [3]:
```

Math functions “magically” loaded.

Basic Python

IPython shell

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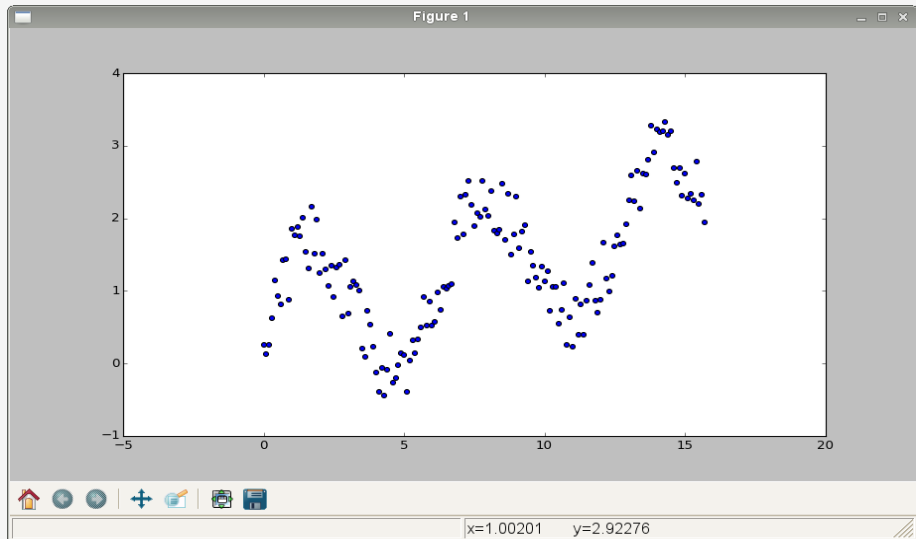
In [3]: scatter(x,y)
Out[3]: <matplotlib.collections.PathCollection at 0x56bdc50>

In [4]: █
```

Plot functions as well.

Basic Python

IPython shell



Basic Python

IPython shell

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In [3]: scatter(x,y)
Out[3]: <matplotlib.collections.PathCollection at 0x5944c50>

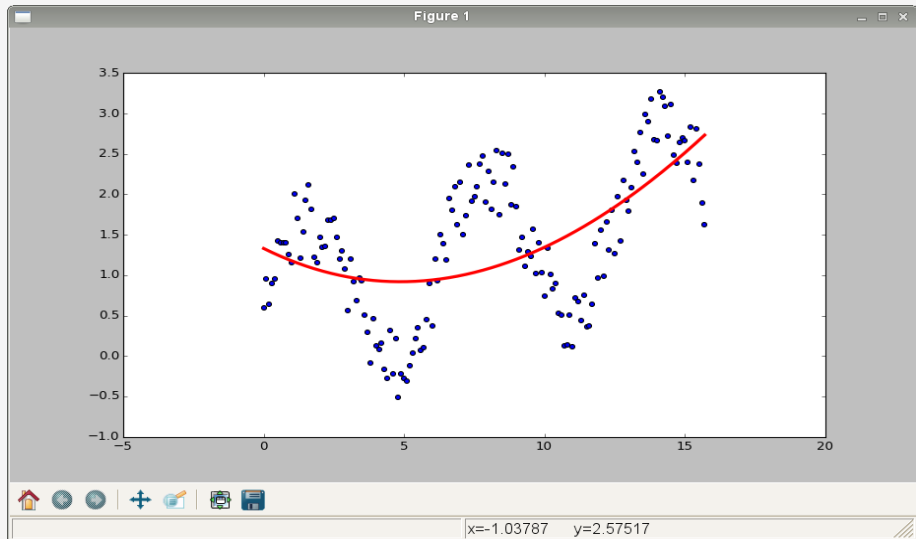
In [4]: fit = polyfit(x,y,3)

In [5]: plot(x, polyval(fit,x), linewidth=3, c="red")
Out[5]: [<matplotlib.lines.Line2D at 0x5959bd0>]

In [6]:
```


Basic Python

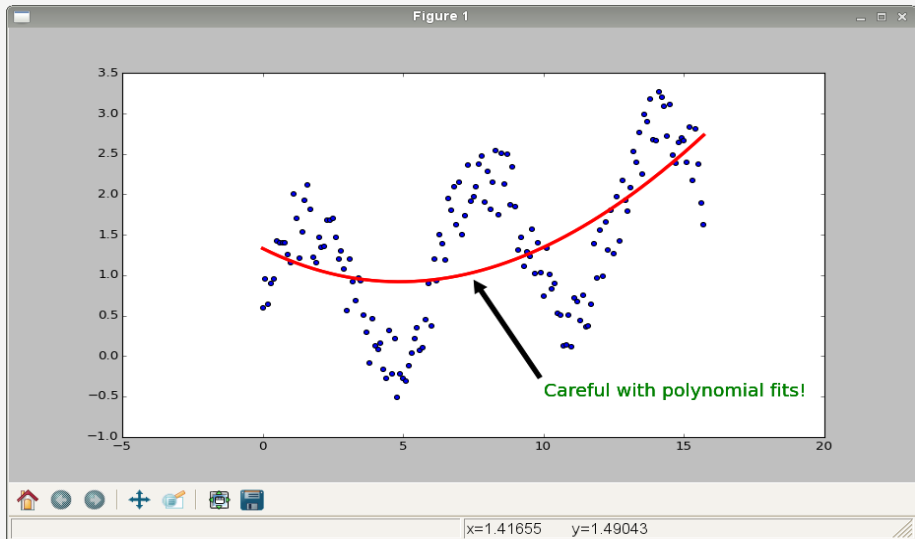
IPython shell



New content can be added interactively.

Basic Python

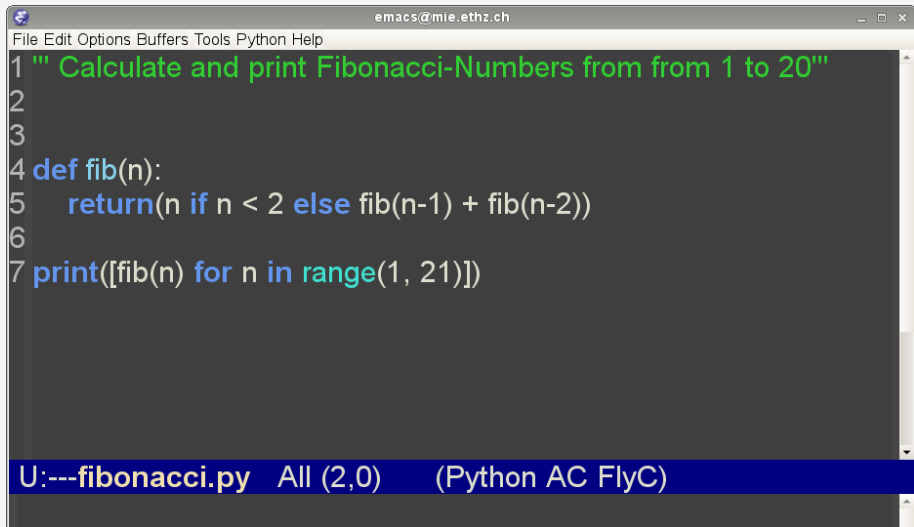
IPython shell



New content can be added interactively.

Basic Python

Run a python script



The screenshot shows an Emacs editor window titled 'emacs@mie.ethz.ch'. The menu bar includes 'File', 'Edit', 'Options', 'Buffers', 'Tools', 'Python', and 'Help'. The code is as follows:

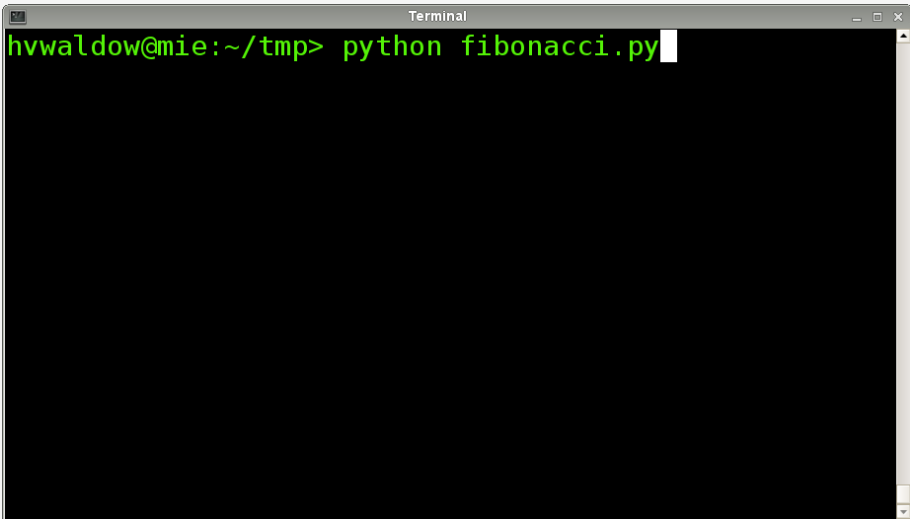
```
1 """ Calculate and print Fibonacci-Numbers from from 1 to 20"""
2
3
4 def fib(n):
5     return(n if n < 2 else fib(n-1) + fib(n-2))
6
7 print([fib(n) for n in range(1, 21)])
```

The status bar at the bottom displays 'U:---fibonacci.py All (2,0) (Python AC FlyC)'.

Save file with ending ".py"

Basic Python

Run a python script

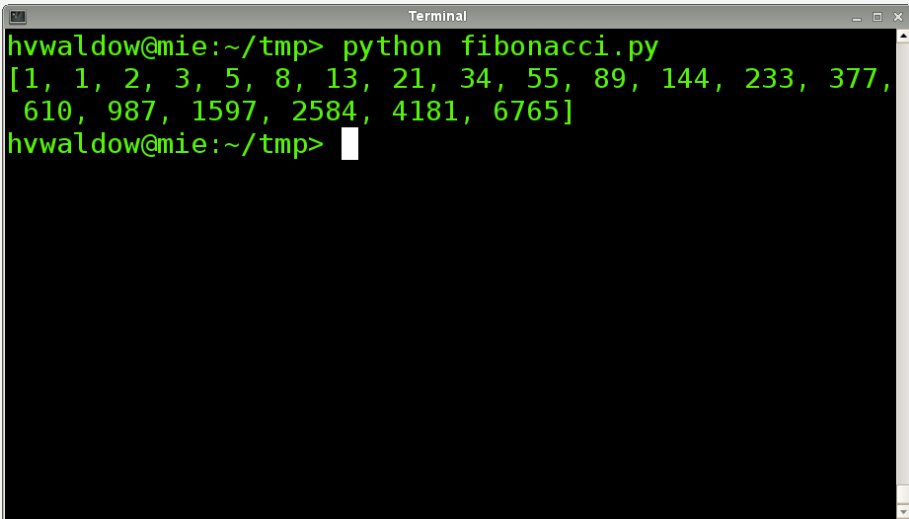
A terminal window titled "Terminal" with a standard macOS-style title bar (red, yellow, green buttons). The terminal has a black background and green text. The prompt is "hvwaldow@mie:~/tmp>". The command "python fibonacci.py" has been entered, and a white cursor is at the end of the line.

```
Terminal
hvwaldow@mie:~/tmp> python fibonacci.py
```

Call python interpreter with filename as argument.

Basic Python

Run a python script

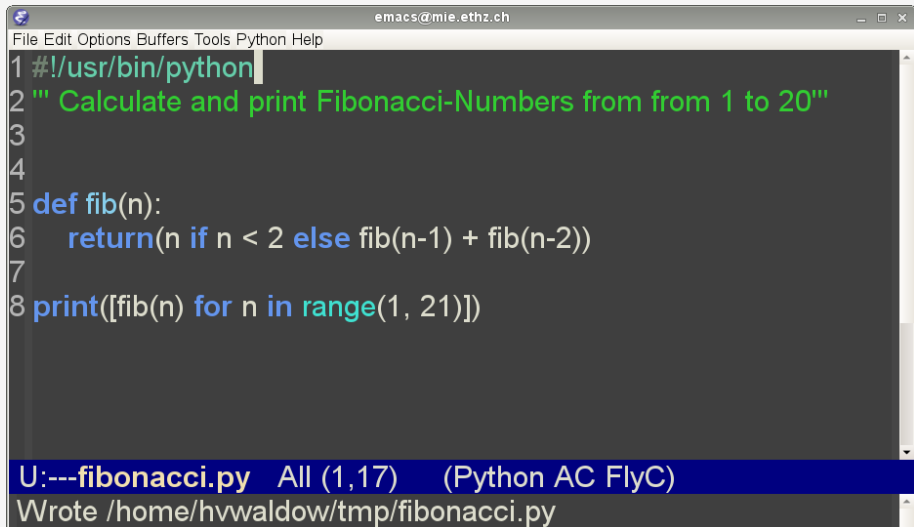
A terminal window titled "Terminal" with standard window controls (minimize, maximize, close) in the top right corner. The prompt is "hvwaldow@mie:~/tmp>". The command "python fibonacci.py" has been entered and executed. The output is a single line of green text: "[1, 1, 2, 3, 5, 8, 13, 21, 34, 55, 89, 144, 233, 377, 610, 987, 1597, 2584, 4181, 6765]". The prompt "hvwaldow@mie:~/tmp>" is followed by a white cursor block.

```
Terminal
hvwaldow@mie:~/tmp> python fibonacci.py
[1, 1, 2, 3, 5, 8, 13, 21, 34, 55, 89, 144, 233, 377,
 610, 987, 1597, 2584, 4181, 6765]
hvwaldow@mie:~/tmp> █
```

Output goes to stdout.

Basic Python

Run a python script



The screenshot shows an Emacs editor window titled 'emacs@mie.ethz.ch'. The menu bar includes 'File', 'Edit', 'Options', 'Buffers', 'Tools', 'Python', and 'Help'. The code is as follows:

```
1 #!/usr/bin/python
2 """ Calculate and print Fibonacci-Numbers from from 1 to 20"""
3
4
5 def fib(n):
6     return(n if n < 2 else fib(n-1) + fib(n-2))
7
8 print([fib(n) for n in range(1, 21)])
```

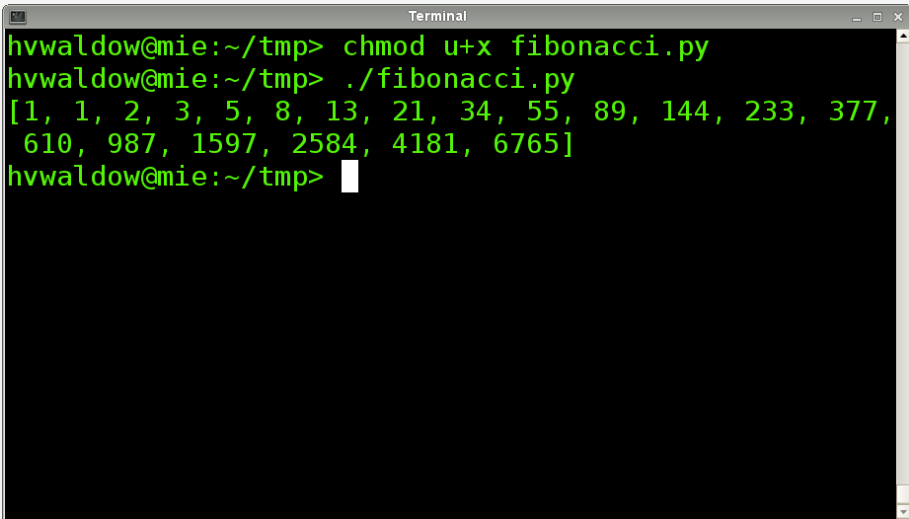
At the bottom of the window, a status bar displays the following information:

U:---fibonacci.py All (1,17) (Python AC FlyC)
Wrote /home/hvwaldow/tmp/fibonacci.py

“Shebang” syntax works.

Basic Python

Run a python script

A terminal window titled "Terminal" with standard window controls. The prompt is "hvwaldow@mie:~/tmp". The user enters "chmod u+x fibonacci.py" and then "./fibonacci.py". The output is a list of Fibonacci numbers: "[1, 1, 2, 3, 5, 8, 13, 21, 34, 55, 89, 144, 233, 377, 610, 987, 1597, 2584, 4181, 6765]".

```
Terminal
hvwaldow@mie:~/tmp> chmod u+x fibonacci.py
hvwaldow@mie:~/tmp> ./fibonacci.py
[1, 1, 2, 3, 5, 8, 13, 21, 34, 55, 89, 144, 233, 377,
 610, 987, 1597, 2584, 4181, 6765]
hvwaldow@mie:~/tmp> 
```

Make script executable and call it directly.

Python development tools

Python IDEs

- A number of sophisticated IDEs available
- Like Matlab, RStudio, Visual Studio, Eclipse ...
- Can be confusing at first
- Many features for program development
- Variable inspection, debugging, ...
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- Spyder (free)

Python development tools

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Python development tools

Python IDEs

The screenshot displays the Spyder Python IDE interface. The main window is titled "Spyder (Python 2.7)". The interface is divided into several panels:

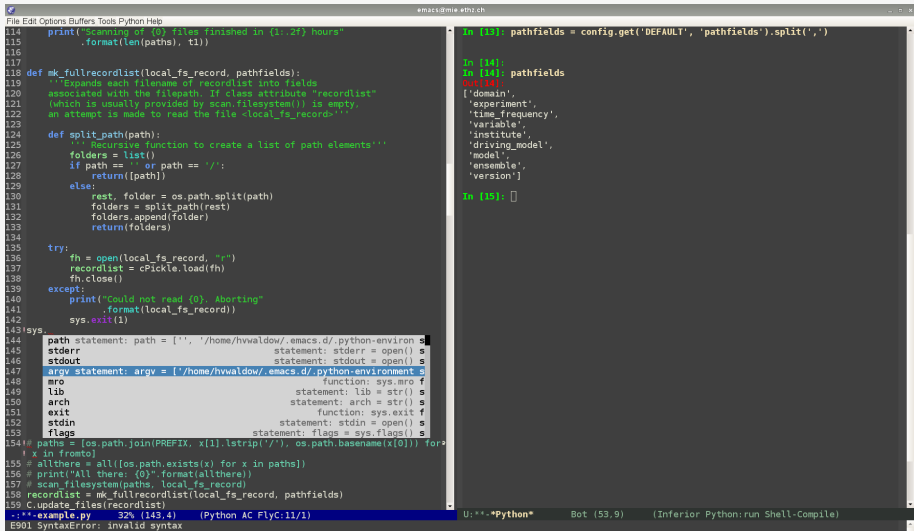
- Editor:** The top-left panel shows a Python script named `temp.py` with the following content:

```
1''' esget fs implements functions that operate mainly in the directory tree
2where ESGET data is stored. Used to find files, examine paths, and move and
3rename files.'''
4
5import logging
6import datetime
7import os
8
9import logging
10import datetime
11import os
12import glob
13from time import ctime
14
15class EsgetFS(object):
16    '''Handles filesystem operations inside the
17    ESGET storage directory-tree'''
18
19    def __init__(self, config):
20        self.fileroot = config.get('DEFAULT', 'fileroot')
21        self.log = logging.getLogger(self.__class__.__name__)
22        self.pathfields = config.get('DEFAULT', 'pathfields').split(',')
23        self.dbname = config.get('Paths', 'dbname')
24        self.wget_tap_dir = config.get('Paths', 'wget_dir')
25        self.wget_log_dir = config.get('Paths', 'wget_log_dir')
26        self.tapdir = config.get('Paths', 'tapdir')
27        self.logfile = config.get('Paths', 'logfile')
28        self.publicdbpath = os.path.join(self.fileroot,
29                                         config.get('Tuning', 'publicdbdir'),
30                                         os.path.basename(self.dbname))
31        self.no_storagefiles = config.get('Tuning',
32                                         'no_storagefiles').split(',')
33
34    def unlink(self, ufiles):
35        '''Moves files to be unlinked into special subdirectory'''
36        if len(ufiles) == 0:
37            self.log.info("No files to unlink")
38            return()
39        curdate = datetime.date.today().isoformat()
40        unlinkpath = os.path.join(self.fileroot, "unlinked", "%04s"
41                                  .format(curdate))
42        os.makedirs(unlinkpath, 0755)
43        if not os.path.exists(unlinkpath):
44            self.log.info("Moving (%d) files into (%s)"
45                          .format(len(ufiles), unlinkpath))
46        self._log.info("Moving (%d) files into (%s)"
47                       .format(len(ufiles), unlinkpath))
48        for f in ufiles:
49            fulpath = os.path.join(unlinkpath,
50                                  os.path.relpath(f, self.fileroot))
51            try:
52                os.rename(f, fulpath)
53            except:
54                self._log.error("Could not unlink (%s)." % f)
55        return()
56
57    def relink(self, unlinkedir):
58        '''Moves previously unlinked files back into main storage-tree'''
59        unlinkpath = os.path.join(self.fileroot, "unlinked", unlinkedir)
60        if not os.path.exists(unlinkpath):
61            self._log.error("Unlinked directory (%s) does not exist" % unlinkpath)
```
- Variable explorer:** The top-right panel shows a table of variables:

| Name | Type | Size | Value |
|-------------|-------|------|--------------------|
| e | float | 1 | 2.718281828459045 |
| euler_gamma | float | 1 | 0.5772156649015329 |
| pi | float | 1 | 3.141592653589793 |
- Object inspector:** The bottom-right panel shows the object inspector, variable explorer, file explorer, and breakpoints.
- Console:** The bottom-left panel shows the console output, including the Python version (2.7.3) and the execution of the `EsgetFS` class.

Python development tools

Editors with plugins



The screenshot shows the Emacs editor interface with a Python script on the left and a REPL on the right. The script defines a function to scan files and a recursive function to split paths. The REPL shows the execution of the script, including the output of the `scan_filesystem` function and the `mk_fullrecordlist` function.

```
File Edit Options Buffers Tools Python Help
114 print("Scanning of {} files finished in {:.2f} hours"
115       .format(len(paths), t1))
116
117
118 def mk_fullrecordlist(local_fs_record, pathfields):
119     '''Expands each filename of recordlist into fields
120     associated with the filepath. If class attribute "recordlist"
121     (which is usually provided by scan.filesystem()) is empty,
122     an attempt is made to read the file <local_fs_record>'''
123
124     def split_path(path):
125         '''Recursive function to create a list of path elements'''
126         folders = list()
127         if path == '' or path == '/':
128             return([path])
129         else:
130             rest, folder = os.path.split(path)
131             folders = split_path(rest)
132             folders.append(folder)
133             return(folders)
134
135     try:
136         fh = open(local_fs_record, "r")
137         recordlist = cPickle.load(fh)
138         fh.close()
139     except:
140         print("Could not read {}. Aborting"
141               .format(local_fs_record))
142         sys.exit(1)
143
144 sys.path.append(os.path.join(PREFIX, x[1].rstrip('/'), os.path.basename(x[0])) for
145                  x in fromto)
146 # all there = all([os.path.exists(x) for x in paths])
147 # print("All there: {}").format(allthere)
148 # scan_filesystem(paths, local_fs_record)
149 recordlist = mk_fullrecordlist(local_fs_record, pathfields)
150 C.update_files(recordlist)
151
152 ***-example.py 32% (143.4) (Python AC FlyC:11/1)
E901 SyntaxError: invalid syntax
```

```
In [13]: pathfields = config.get('DEFAULT', 'pathfields').split(',')
In [14]:
Out[14]:
['domain',
 'experiment',
 'time_frequency',
 'variable',
 'institute',
 'driving_model',
 'model',
 'ensemble',
 'version']
In [15]:
```

Python development tools

Editors with plugins

- Emacs
- Vim
- other editors with varying degrees of support
- Geany, TextWrangler, ...
- More screen-estate for code & interpreter
- Keyboard instead of mouse \Rightarrow faster!
- Might be complicated to set up, initially.
- Steeper learning curve
- If you already use Emacs or Vim, go for it!

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Python development tools

And now for something completely different ...



Learning and teaching Python in the 21st century

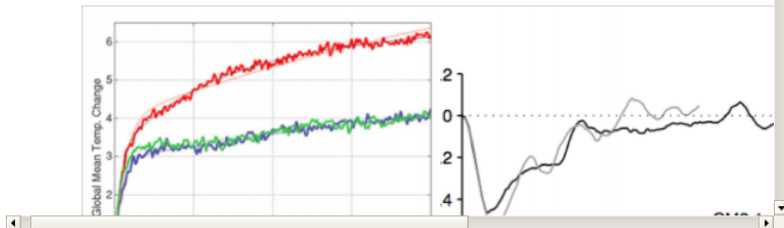
```
In [6]: from IPython.display import IFrame  
IFrame('http://www.gfdl.noaa.gov/blog/isaac-held/', width='100%', height=300)
```

Out[6]:



50. Volcanoes and the Transient Climate Response - Part II

Posted on [September 3, 2014](#) by [Isaac Held](#)



Mr. Crezee, übernehmen Sie!