Ten years of (interactive) scientific Python

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EuroScipy 2011,
Ecole Normale Supérieure, Paris.
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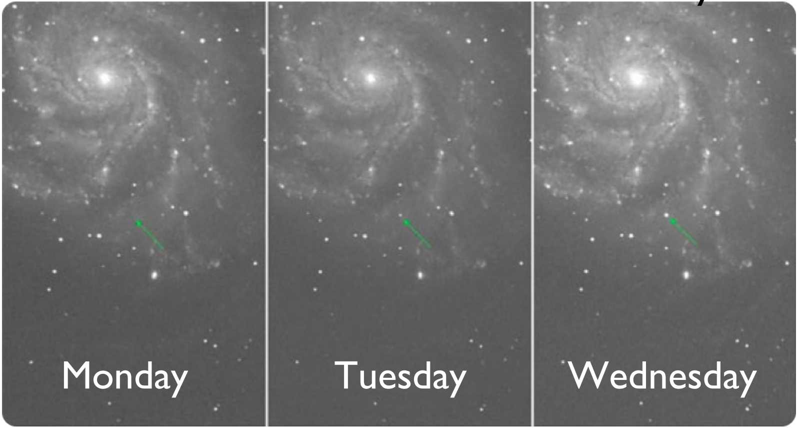
BREAKING
NEWS

Supernova PTF11kyl:

Event of a Generation found on Tuesday



Most nearby Type Ia supernova in > 25 years

Soon visible with binoculars

http://bit.ly/ptf11kly

Astronomy Challenge:

Quickly find new events in millions of (mostly bogus) candidates/night

Palomar Transient Factory (2009-now)

Solution:

Train a machine to mimic expert labels

- **Python Google App Engine** used for training
- **scipy** for expert voting
- **Jython** to run machine-learning on new data

➜1000 to 1 compression allows PTF to focus on most probable candidates

arXiv.org > astro-ph > arXiv:1106.5491

Bloom et al. 2011

Outline

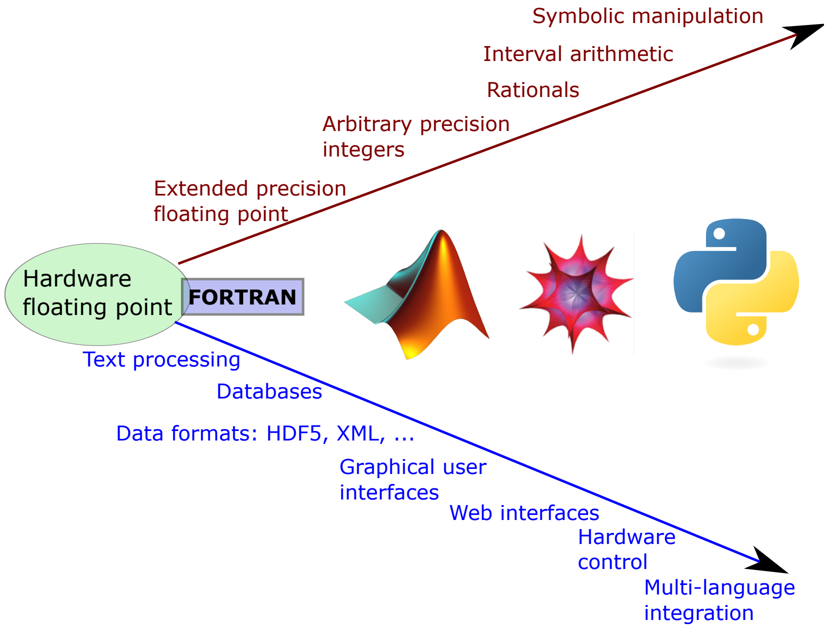
Outline

Science and computing: a changing landscape

- High level systems: beyond C and Fortran
- The data avalanche
- Massive resources at low cost
- Internet: enabler of Open Source Software
  - development model akin to scientific traditions
  - viable alternatives to proprietary software

Computing is not the 'third branch' of science...

It is now the backbone of theory *and* experiment!

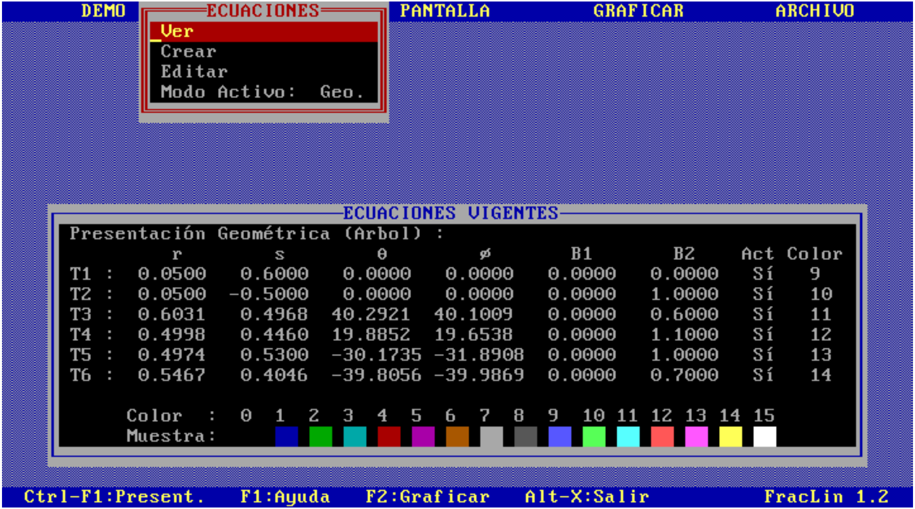

Symbolic manipulation
Interval arithmetic
Rationals
Arbitrary precision integers
Extended precision floating point
Hardware floating point
FORTRAN
Text processing
Databases
Data formats: HDF5, XML, ...
Graphical user interfaces
Web interfaces
Hardware control
Multi-language integration

Me? No real training in computing

- High school in Colombia, the 80's
  - TI-99/4A, 16KB Basic, home Sony tape recorder.
  - A few home tutoring lessons on 'structured programming', promptly forgotten.
    - Never did anything interesting.
- College in Colombia, EE:
  - One semester of Pascal; my only formal computer course ever.

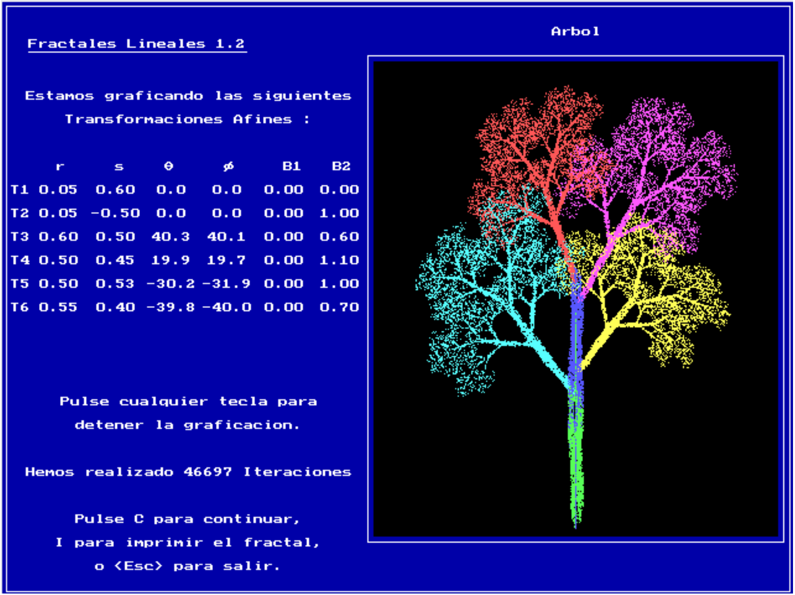
Switch to physics, plot fractals in TurboPascal

- Program on paper, use mom's office PC on weekends.
- Debug on paper. Think a lot away from the screen.



VGA graphics!

Binary compiled in 1991/92, screenshot taken May 2011!



Clueless about the internet (which I unplugged)

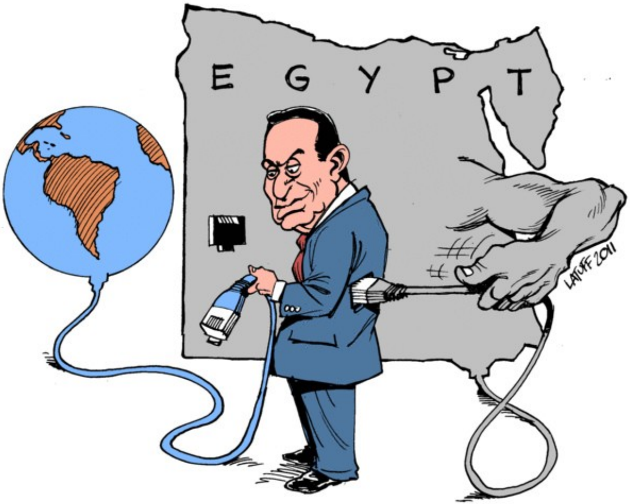


Image credit: Carlos Latuff

A learning moment...

Image credit: crazytales562 on Flickr

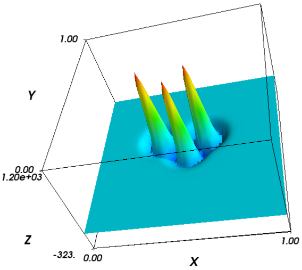
High-level tools are important

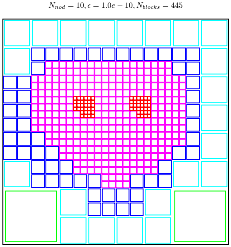
- Undergraduate thesis: the electrostatic unrestricted 3-body problem.
    - Maple ⇒ C ⇒ Gnuplot.
    - Code generation as a natural part of the problem
    - Multi-language integration.
- Teach computational physics for undergrads: C/Gnuplot on VAX talking to a 486PC running Linux.
    - A complete disaster.
    - Never again! Need different/better tools.
- Thesis at CU Boulder: lattice QCD (numerical Quantum Chromodynamics)
    - large open source C package (MILC),
    - custom C code, Mathematica, IDL, bash, sed, awk, Perl, Gnuplot. (*)
- End of my PhD: Python.
    - **Big revelation: all of (*) ⇒ One language!!!**

Postdoc work: Adaptive, multiwavelet PDE tools

Gregory Beylkin, Vani Cheruvu, FP. Applied Math, CU Boulder.

- Fast application of integral kernels. (Partial Differential Equations)
- Jump from 1 to 3 dimensions: *extremely unusual*
- Complex algorithm: beyond numerics.
- Performance: to NumPy, F2PY, weave.
    - Dynamically generated C++ sources: code as a run-time resource.





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Why IPython?

(something other than
"I'd rather not finish my dissertation")

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I is for interactive...

In scientific computing,
we typically don't know what we're doing.

Scientific computing $\Leftrightarrow$ *Exploratory* computing

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Interactive systems

Features

- **Execute/explore cycle instead of edit/compile/run**
- **Rich Libraries**
- **Plotting and data visualization**

Examples

- **Mathematica/Maple:** symbolic, now numerics...
- **IDL/Matlab:** numerics, image processing, ...
- **Unix system shell:** file management/text processing.

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Python: an excellent *base* for an interactive scientific system

- Dynamic code evaluation
- No variable declarations
- Powerful introspection
- Very regular object model
- Excellent string processing

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I said *a base*...

/bin/bash

```
dreamweaver[~]> python
Python 2.6.6 (r266:84292, Sep 15 2010, 16:22:56)
[GCC 4.4.5] on linux2
Type "help", "copyright", "credits" or "license" for more information.
>>> ls
Traceback (most recent call last):
  File "<stdin>", line 1, in <module>
NameError: name 'ls' is not defined
>>> 
```

Mmh, introspection?

```
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Basic comforts?

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>>> execfile('~/scratch/err.py')
Traceback (most recent call last):
  File "<stdin>", line 1, in <module>
IOError: [Errno 2] No such file or directory: '~/scratch/err.py'
>>> 
```

Useful error info

/bin/bash

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Traceback (most recent call last):
  File "<stdin>", line 1, in <module>
IOError: [Errno 2] No such file or directory: '~/scratch/err.py'
>>> execfile('/home/fperez/scratch/err.py')
Traceback (most recent call last):
  File "<stdin>", line 1, in <module>
  File "/home/fperez/scratch/err.py", line 9, in <module>
    foo33
NameError: name 'foo33' is not defined
>>>
>>> 
```

We can do better...

My files, thankyouverymuch

```
/bin/bash
dreamweaver[~]> ipython
Python 2.6.6 (r266:84292, Sep 15 2010, 16:22:56)
Type "copyright", "credits" or "license" for more information.

IPython 0.11.dev -- 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]: ls ~/scratch/er*py
/home/fperez/scratch/err25.py      /home/fperez/scratch/error.py*
/home/fperez/scratch/err_comps.py  /home/fperez/scratch/err.py

In [2]: 
```

Some object details?

```
Type:           module
Base Class:     <type 'module'>
String Form:    <module 'os' from '/usr/lib/python2.6/os.pyc'>
Namespace:      Interactive
File:           /usr/lib/python2.6/os.py
Docstring:
    OS routines for Mac, NT, or Posix depending on what system we're on.

    This exports:
      - all functions from posix, nt, os2, or ce, e.g. unlink, stat, etc.
      - os.path is one of the modules posixpath, or ntpath
      - os.name is 'posix', 'nt', 'os2', 'ce' or 'riscos'
      - os.curdir is a string representing the current directory ('.' or ':')
      - os.pardir is a string representing the parent directory ('..' or '::')
      - os.sep is the (or a most common) pathname separator ('/' or ':' or '\\')
      - os.extsep is the extension separator ('.' or '/')
      - os.altsep is the alternate pathname separator (None or '/')
      - os.pathsep is the component separator used in $PATH etc
      - os.linesep is the line separator in text files ('\r' or '\n' or '\r\n')
      - os.defpath is the default search path for executables
      - os.devnull is the file path of the null device ('/dev/null', etc.)

    Programs that import and use 'os' stand a better chance of being
lines 1-23
```

More info??

/bin/bash

```
Type:           module
Base Class:     <type 'module'>
String Form:    <module 'code' from '/usr/lib/python2.6/code.pyc'>
Namespace:      Interactive
File:           /usr/lib/python2.6/code.py
Source:
"""Utilities needed to emulate Python's interactive interpreter.

"""

# Inspired by similar code by Jeff Epler and Fredrik Lundh.


import sys
import traceback
from codeop import CommandCompiler, compile_command

__all__ = ["InteractiveInterpreter", "InteractiveConsole", "interact",
           "compile_command"]

def softspace(file, newvalue):
    oldvalue = 0
    try:
        oldvalue = file.softspace
    except AttributeError:
        pass
    try:
        file.softspace = newvalue
lines 1-28
```

When things go wrong

```
/bin/bash

In [13]: run ~/scratch/error
reps: 5
---------------------------------------------------------------------------
ValueError                                Traceback (most recent call last)
/home/fperez/scratch/error.py in <module>()
     70 if __name__ == '__main__':
     71     #explode()

---> 72     main()
     73     g2='another global'

/home/fperez/scratch/error.py in main()
     60     array_num = zeros(size,'d')
     61     for i in xrange(reps):
---> 62         RampNum(array_num, size, 0.0, 1.0)
     63     RNtime = time.clock()-t0
     64     print 'RampNum time:', RNtime

/home/fperez/scratch/error.py in RampNum(result, size, start, end)
     43     tmp = zeros(size+1)
     44     step = (end-start)/(size-1-tmp)
---> 45     result[:] = arange(size)*step + start
     46
     47 def main():

ValueError: shape mismatch: objects cannot be broadcast to a single shape

In [14]:
```

ipython --pylab

fperez@longs:/home/fperez - Shell - Konsole

```
longs[~]> ipython -pylab
Python 2.4.3 (#2, Apr 27 2006, 14:43:58)
Type "copyright", "credits" or "license" for more information.

IPython 0.7.3.svn -- An enhanced Interactive Python.
?       -> Introduction to IPython's features.
%magic  -> Information about IPython's 'magic' % functions.
help    -> Python's own help system.
object? -> Details about 'object'. ?object also works, ?? prints more.

  Welcome to pylab, a matplotlib-based Python environment.
  For more information, type 'help(pylab)'.

In [1]: import math, numpy

In [2]: from scipy.integrate import quad

In [3]: from scipy.special import j0

In [4]: def j0i(x):
   ...:     """Integral form of J_0(x)"""
   ...:     def integrand(phi):
   ...:         return math.cos(x*math.sin(phi))
   ...:     return (1.0/math.pi)*quad(integrand,0,math.pi)[0]
   ...:

In [5]: x = numpy.linspace(0,20,200) # sample grid: 200 points between 0 and 20

In [6]: y = j0(x)  # sample J0 at all values of x

In [7]: x1 = x[::10]  # subsample the original grid every 10th point

In [8]: y1 = map(j0i,x1)  # evaluate the integral form at all points in x1

In [9]: # Make a plot with these values (the ; suppresses output)

In [10]: plot(x,y,label=r'$J_0(x)$');

In [11]: plot(x1,y1,'ro',label=r'$J_0^{\textrm{integ}}(x)$');

In [12]: axhline(0,color='green',label='_nolegend_');

In [13]: title(r'Verify $J_0(x)=\frac{1}{\pi}\int_0^{\pi}\cos(x \sin\phi)\,d\phi$');

In [14]: xlabel('$x$');

In [15]: legend();

In [16]: matshow(numpy.random.random((32,32)))
Out[16]: <matplotlib.figure.Figure instance at 0x4630042c>
```

Shell

Figure 1

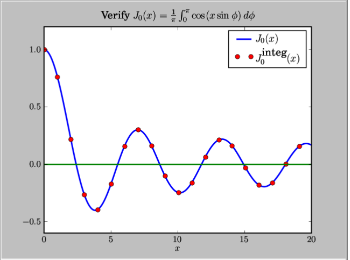
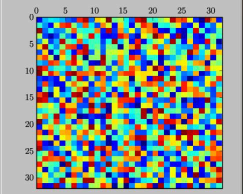
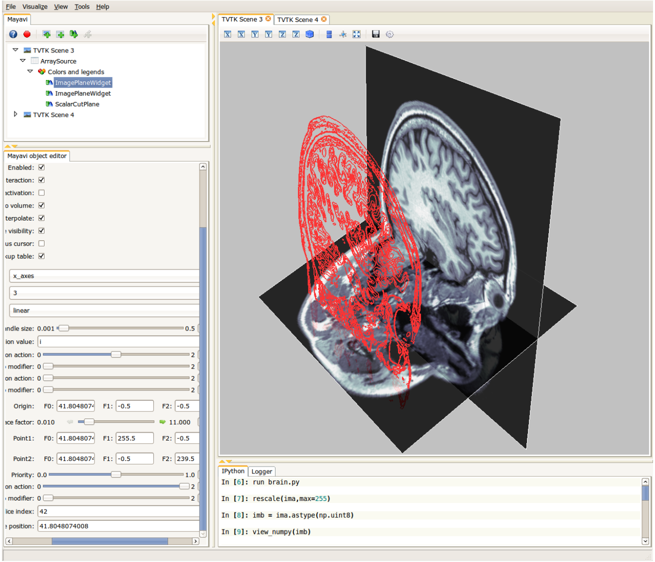


Figure 2



Embedded widget



- **October/November 2001: “just a little afternoon hack“**
  - My own `$PYTHONSTARTUP` hack:
    - `ipython-0.0.1.py`: 259 lines.
    - Mathematica’s `In [N]:` prompts and `%N` results cache.
  - IPP (Interactive Python Prompt) by Janko Hauser (Oceanography)
  - LazyPython by Nathan Gray (CS Caltech)
- **2002: Ignore John Hunter’s Gnuplot support patches**
  - ... let there be matplotlib
  - and the world rejoyced.
  - (actually finish my PhD!)

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  Physics @ U. Santa Clara
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  - Min's senior undergrad thesis (Physics @ U. Santa Clara, CA):
    - first parallel tools, Twisted-based
- **2005: Ville Vainio**
  - Core maintenance while we worked on machinery for parallelism.
- **2008: Gaël Varoquaux/Enthought: `ipythonx`**
  - WX widget: standalone and embeddable (MayaVi)
- **2008: Laurent Dufréchou: `ipython-wx`**
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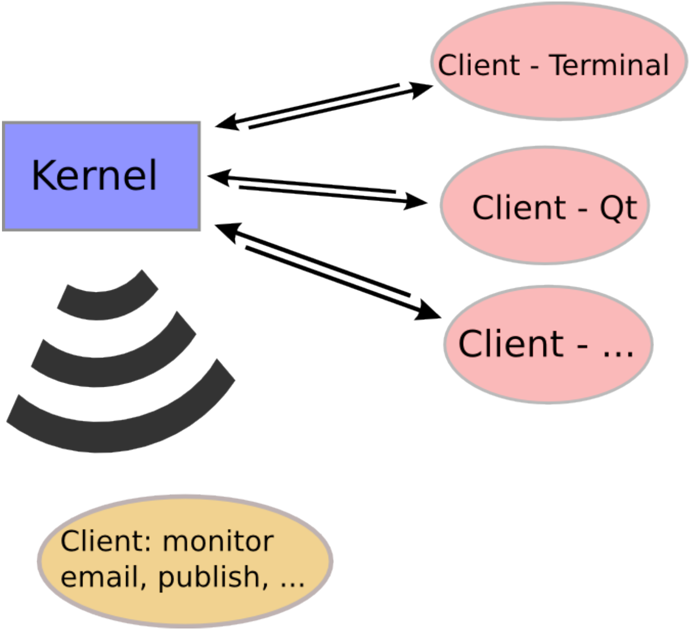
More complex interactive uses?



A messaging protocol

Direct communication

- Execute code ('eval')
- Object information
- Complete
- History
- Connect

Broadcasting

- Functional execution:
  - Python inputs
  - Python outputs
  - Python errors
- Side effects:
  - Streams (stdout, stderr, etc)
  - Display data: plots, other payloads

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ØMQ - "Sockets done right"

http://zeromq.org

The socket library that acts as a concurrency framework

- Pure C++ library.
- Python bindings in Cython (Brian Granger, Min RK). Python 2.5-3.2.
- Python bindings run messaging in native threads - no GIL
- Abstractions are at the message delivery level, not the raw-bytes level.
- Socket types encapsulate messaging patterns.
- Open source (LGPL), actively developed.

ØMQ: Messaging *patterns*

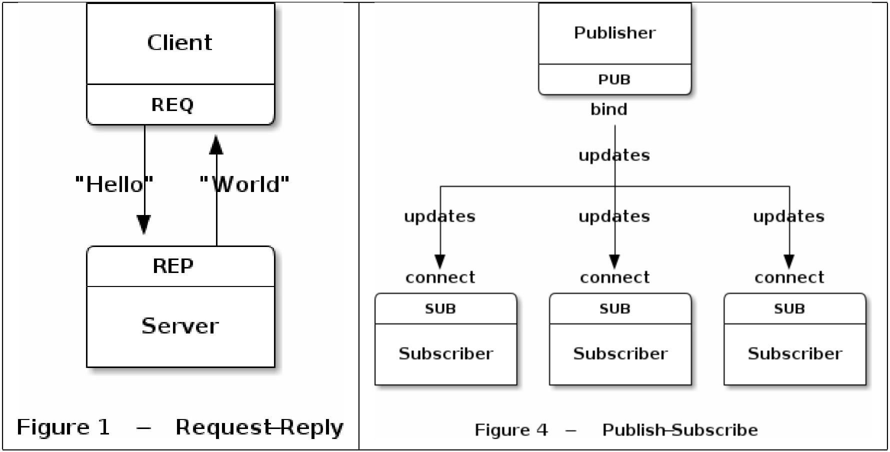

Image credit: official ØMQ documentation

A bit more history: 2010

- **February: discover ØMQ (ZeroMQ)**
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- **March: proof of concept of shell over ØMQ**
  - 2-day sprint with Brian
  - Simple, clean, performant. We're thrilled.
- **May: switch from Bazaar/Launchpad to Git/Github**
  - Learn Git NOW.
  - Github rocks. Seriously.
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2010 Summer/Fall

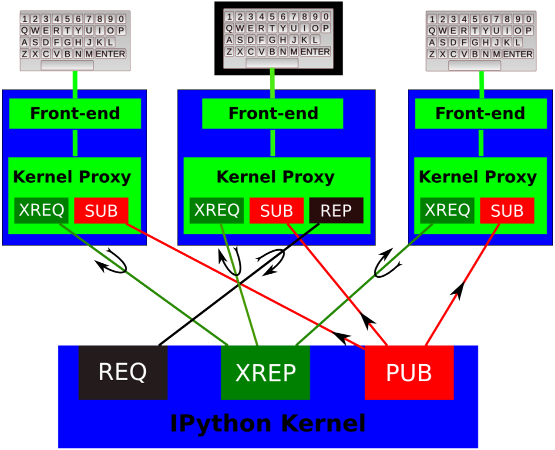
Enthought sponsorhip, things kick into high gear.

- **Rich Qt Console**
  - Evan Patterson (Caltech physics)
- **Full kernel over ØMQ**
  - Brian Granger (now at Cal Poly San Luis Obispo physics) and FP.
- **Implement parallel machinery over ØMQ**
  - Min Ragan-Kelley (now at UC Berkeley, plasma physics)
  - (btw, this is *insane* – though par for the course for Min)
- **HTML/JavaScript frontend: the web notebook was coming**
  - James Gao (UC Berkeley neuroscience)
- **Python 3 port of core terminal code**
  - Thomas Kluyver

2011

- **Release 0.11**
  - Qt console
  - ZeroMQ parallel code
  - Removed all Twisted code
  - The start of the path to IPython 1.0
- **Develop the web notebook**
  - Summer: Brian codes like mad
  - Built on the same architecture
- **Full Python 3 support**

An architecture for interactivity with ØMQ



- Kernel raw_input

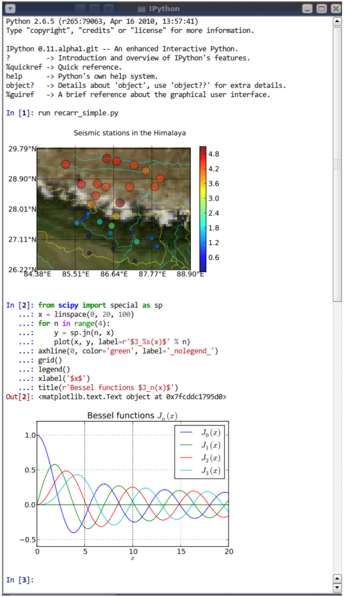
- Requests to kernel

- Kernel output broadcast

- Request/Reply direction

Client: a rich Qt Console

Enthought: sponsorship, Evan Patterson, Robert Kern.

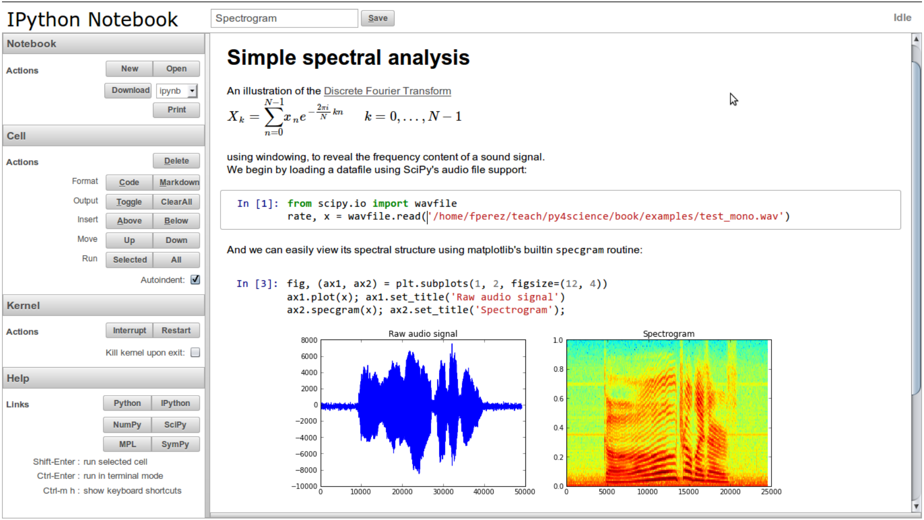


Feels like a console, runs like a GUI

- Inline and floating images
- Syntax highlighting, full multiline editing
- Session saving
  - HTML (with PNG or SVG)
  - PDF/printing
- Help viewer
- %magics, `!system access`, IPython...
- Detach/reattach support

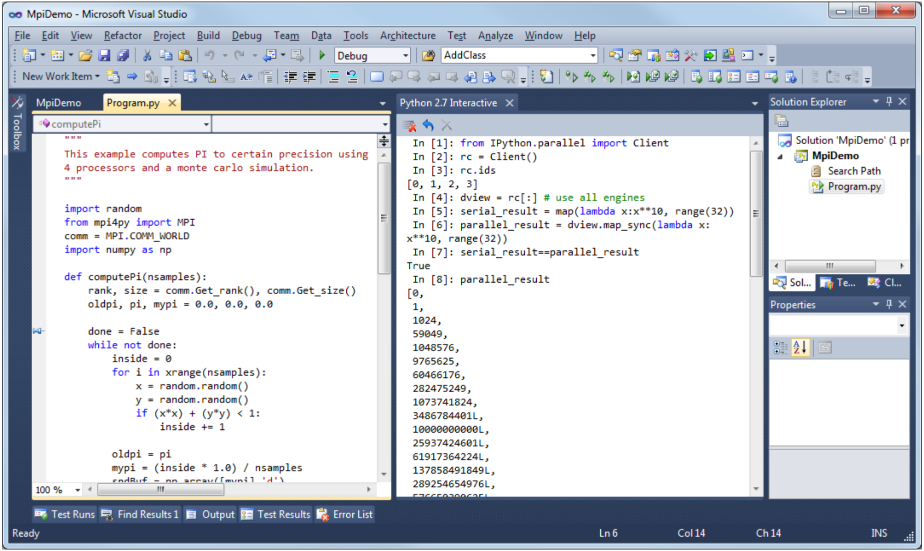
Client: a web notebook

Brian Granger, James Gao.



Client: Microsoft Visual Studio 2010

Dino Viehland and Shahrokh Mortazavi; http://pytools.codeplex.com



Other projects using IPython

Scientific

- **Sage**: open source mathematics.
- **PyRAF**: Space Telescope Science Institute
- **CASA**: Nat. Radio Astronomy Observatory
- **Ganga**: CERN
- **PyMAD**: neutron spectrom., Laue Langevin
- **Sardana**: European Synchrotron Radiation
- **ASCEND**: eng. modeling (Carnegie Mellon).
- **JModelica**: dynamical systems.
- **DASH**: Denver Aerosol Sources and Health.
- **PyIMSL** Studio, by Visual Numerics.
- **Trilinos**: Sandia National Lab.
- **Pymerase**: microarray gene expression.
- **DoD**: baseline configuration.
- **Mayavi**: 3d visualization, Enthought.
- **NiPype**: computational pipelines, MIT.
- **QSnake**: source-distro for scientific comp.

Web/Other

- **Visual Studio 2010**: MS.
- **Django** web.
- **Turbo Gears** web.
- **Pylons** web framework
- **Zope** and **Plone** CMS.
- Axon Shell, BBC **Kamaelia**.
- **Schevo** database.
- **Pitz**: distributed task/bug tracking.
- **iVR** (interactive Virtual Reality).
- **Movable Python** (portable Python environment).
- ...

(Incomplete) Cast of Characters

- **Brian Granger**- Physics, Cal State San Luis Obispo
- **Min Ragan-Kelley** - UC Berkeley
- **Thomas Kluyver** - U. Sheffield
- **Evan Patterson**- Caltech/Enthought
- **Robert Kern** - Enthought
- **Jörgen Stenarson** - SP Technical Research Institute of Sweden.
- Ondrej Certik - Physics, U Nevada Reno
- Darren Dale - Cornell
- Laurent Dufréchou - France
- James Gao - UC Berkeley
- Satra Ghosh- MIT Neuroscience
- John Hunter - TradeLink Securities, Chicago.
- Paul Ivanov - UC Berkeley
- Prabhu Ramachandran - Aerospace Engineering, IIT Bombay.
- Justin Riley - MIT
- Thomas Spura - Fedora project
- Ville Vainio - CS, Tampere University of Technology, Finland
- Stefan van der Walt - Applied Math, U. Stellenbosch, South Africa
- Gaël Varoquaux - Neurospin (Orsay, France)
- Mark Voorhies - UC San Francisco
- Many more! (~60 commit authors)

- **Enthought**, Austin, TX: **Lots!**
- Tech-X Corporation, Boulder, CO: Parallel/notebook (previous versions)
- Microsoft: WinHPC support, Visual Studio and Azure integration
- NIH: via NiPy grant
- NSF: via Sage compmath grant
- Google: summer of code 2005, 2010.

Hands-on

Outline

1. Personal view of scientific computing
2. IPython
3. Rethinking interactivity
4. The IPython Notebook
5. Parallelism?
6. Trouble in paradise

We're very excited

- **Capturing exploratory workflows (for self or others)**
    - Reproducibility in research
- **Interactive documents**
    - Mathematica `Manipulate`, Sage `@interact`.
- **Teaching**
    - Tutorials and documentation
- **Publication:** Papers and books
- **A rich document format and API**
- **Very long list of ideas...**

We really want community buy-in, hence critical feedback!

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Outline

The infamous Global Interpreter Lock in CPython

Only one thread can modify Python state/variables at a time

- Historical reasons, simplicity of implementation
- All attempts at removing it have failed
- Threads useless for CPU-bound problems.

The best possible reference on the GIL: David Beazley's work

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IPython: a REPL (Read/Eval/Print Loop)

Core idea: manage a namespace

- Read: take user input.
- Eval: execute code.
- Print: provide output.
- Add support for data transfer...

...and interactive and parallel work start looking very similar.

These steps can happen in multiple processes:

- Read: user environment
- Eval: kernel process
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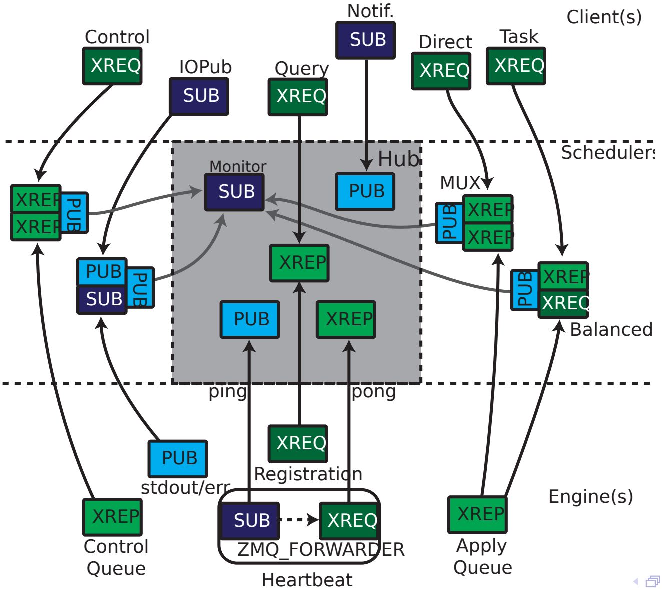

Notif.
SUB
Client(s)
Control
XREQ
Direct
XREQ
Task
XREQ
IOPub
SUB
Query
XREQ
Hub
Schedulers
Monitor
SUB
PUB
MUX
XREP
XREP
PUB
PUB
XREP
XREP
PUB
PUB
SUB
PUB
XREP
PUB
XREP
XREQ
PUB
PUB
XREP
Balanced
ping
pong
XREQ
Registration
PUB
stdout/err
Engine(s)
SUB
XREQ
ZMQ_FORWARDER
Heartbeat
XREP
Control
Queue
XREP
Apply
Queue

A few simple concepts

- The **client**: lightweight handle on all engines of a cluster
- The **views**: "slice" the client with specific execution semantics
  - `DirectView`: direct execution on *all* engines (blocking or not)
  - `LoadBalancedView`: run on *any one* engine.
- `x.apply()`: highly functional API.
- `AsyncResult`: similar to the one in `multiprocessing`.
- The **controller**: manage all activity in a cluster (accessed via *clients*)

Multiple usage patterns

- Direct interface: explicit (and flexible) control of where things run.
    - Choice of blocking behavior up to the user.
- Task interface: load-balanced (with flexible scheduling policies)
- Data push/pull, scatter/gather.
- Decorators that encapsulate many common patterns
- Informative exception propagation
- Explicit node-to-node communication:
    - MPI-style problems
    - ... without all the pain of MPI.

Hands-on

Neat trick: DAG dependencies

A simple DAG example

```
In [2]: G = random_dag(32,128)
In [3]: jobs = {}

# in reality, each job would presumably be different
# randomwait is just a function that sleeps for a random interval
In [4]: for node in G:
   ...:     jobs[node] = randomwait

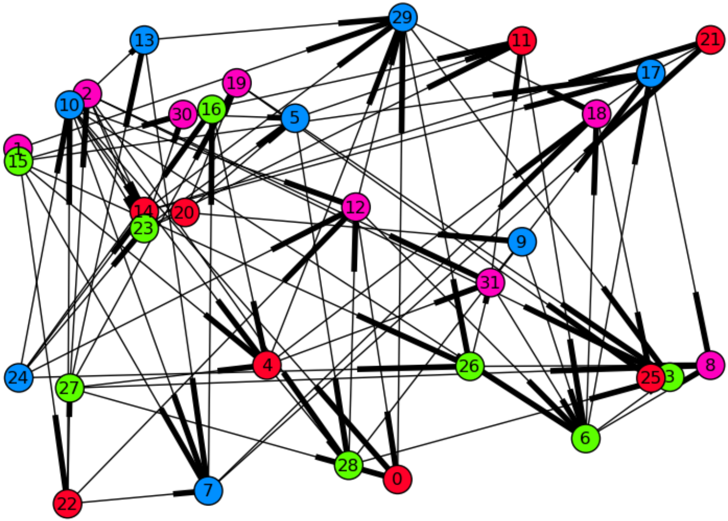
In [5]: c = client.Client()

In [6]: results = {}

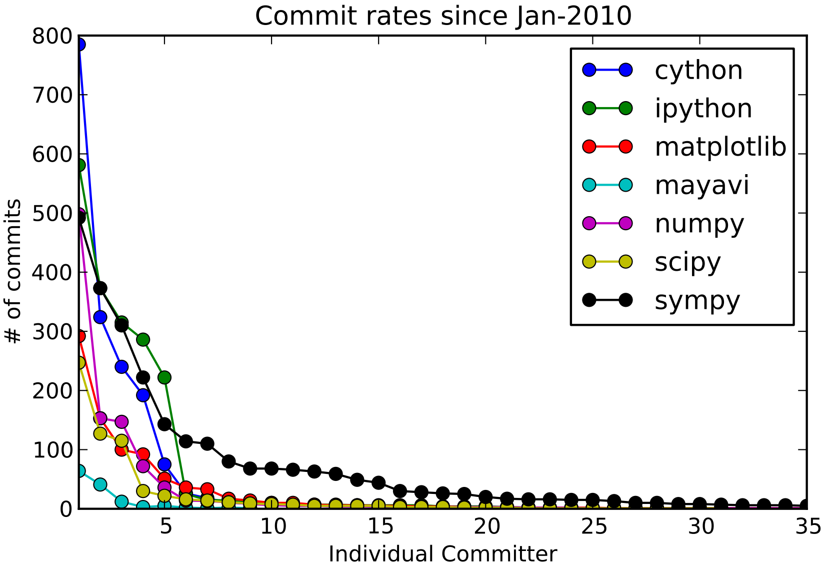
In [7]: for node in G.topological_sort():
   ...:     # get list of AsyncResult objects from nodes
   ...:     # leading into this one as dependencies
   ...:     deps = [ results[n] for n in G.predecessors(node) ]
   ...:     # submit and store AsyncResult object
   ...:     results[node] = client.apply(jobs[node], after=deps,
     block=False)

In [8]: [ r.get() for r in results.values() ]
```

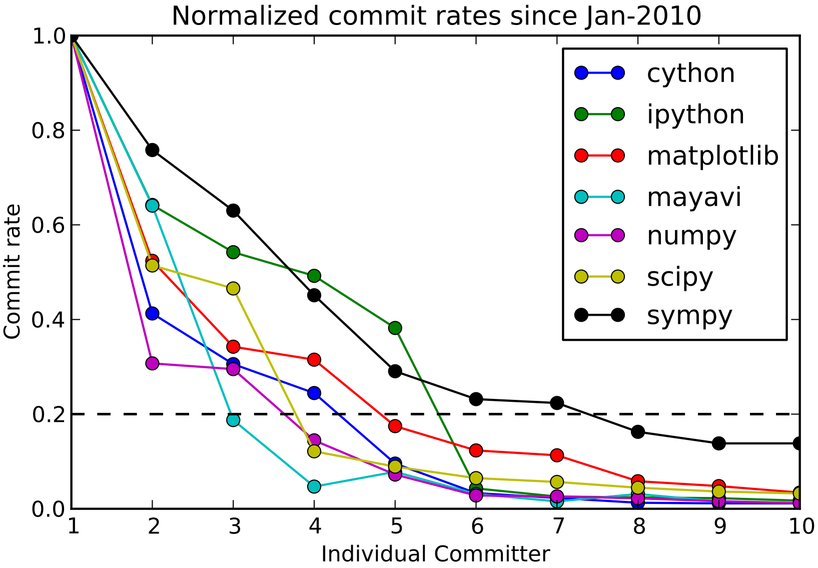
DAG dependencies - validation



Outline



Commit rates since Jan-2010
# of commits
Individual Committer
0
100
200
300
400
500
600
700
800
5
10
15
20
25
30
35
cython
ipython
matplotlib
mayavi
numpy
scipy
sympy



Normalized commit rates since Jan-2010
Commit rate
Individual Committer
cython
ipython
matplotlib
mayavi
numpy
scipy
sympy

We have problems

Python in science is a great success story, but...

The entire edifice rests on (often the spare time of) ~30 people!

- A backbone of top-heavy projects
- Formal funding hard to come by
  - Glimmers of hope, e.g. Ed Seidel @ NSF.
- Software work in science can be career suicide.

Not a sustainable strategy for the long term

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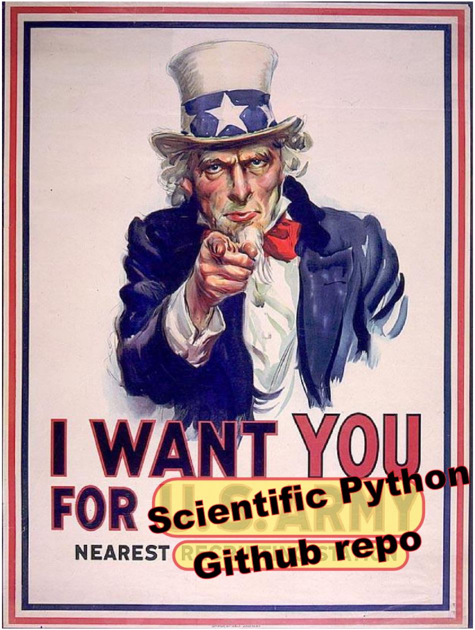
I WANT YOU
FOR
Scientific Python
NEAREST
Github repo

How can you help?

- **Teach a class?**
  - Real world homework projects!
- **Tenure/grant panel?**
  - Don't kill candidates who contribute software
  - **Do** kill proposals who pay lip service to real development work
- **Have your own project?**
  - Put it up on Github, BSD/MIT license it
- **Just join in!**
  - Work on whatever project interests **you**.

Plenty of interesting problems

- **IPython**
  - Reproducible research, interactive documents, parallel APIs, MPI for the rest of us, from notebook to paper, ...
- **Numpy**
  - multidimensional data descriptions, array VMs, database interactions, jagged arrays, streaming access, ...
- **Matplotlib**
  - grammar of graphics, streaming data, Javascript interactivity, beyond the Matlab API, ...
- **Scipy**
  - Sparse tensors, adaptive functional interpolators, statistics (with sk.learn, statsmodels), code generation models, ...
- **Python itself**
  - new operators (PEP 225), decimals and rationals, docstrings, the packaging hell, ...

The incentive structure of academia fits poorly

the widely distributed,

rapid-fire collaborative dynamics

of open source development

Aside - BSD/MIT licenses?

- The GPL: a good tool for applications (Linux kernel)
- Bad for libraries:
  - Infinite leverage
- A spirit of reciprocity
  - You are building on millions of lines of BSD-type code
  - GPL code is worse than closed source as a contribution to those foundations
- We have been well served by permissive licensing
  - 10 years of productive engagement with industry
- Nobody is going to get rich by 'stealing' your code
  - Building a successful business takes MUCH more than putting a price sticker on a piece of code.

In closing

- The **language** lured me in...
- But I stayed for the **community**!
  - Real **friendships** and incredible people
  - A culture of generous and mutual cross-project **collaboration**
  - But we have a **ton of work** to do!
- The tools we need **must be built by scientists.**

Lots of space for truly innovative thinking, and Python is an expressive tool for the exercise.

Thank you!

Questions?