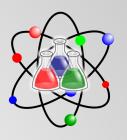


Developing a scientific software library (... and spreading the word)

Tobias Megies, Lion Krischer (...)
June 2014

Software in Science



- Going from research code to distributable and reusable code easily is 5-10 times as expensive
- Gain in hard research currency (e.g. publications) is questionable

WHY DO IT?

- Science needs it and the need will only increase
- Helps the whole community no need to do it 100 times (quickly? badly?) if done once but properly
- In the long run, if embraced by all, greatly reduces the time to research for all
- Helps with reproducibility a still unsolved issue

Software in Science - Issues



- Software development skills
 - Not a thoroughly taught skill but many of us spend a lot of time doing it.
- Sustainability
 - How to keep it going after the project finishes?
- Community building
 - Good software without users has little value. How to spread the word?
- Limited resources in money and time
 - Most scientific software is a by-product of actual research; very little funding for software developments.
- Recognition and rewards
 - Not the same value as publications and hard to build an academic career from it.

Outline

- 1. Introduction to Python and ObsPy
 - a. Why Python?
 - b. Functionality of ObsPy
 - c. Basic Usage Examples
- 2. Some Technical Details
 - a. Testing
 - b. Code Management and Communication
- 3. "spreading the word"

Why Python?



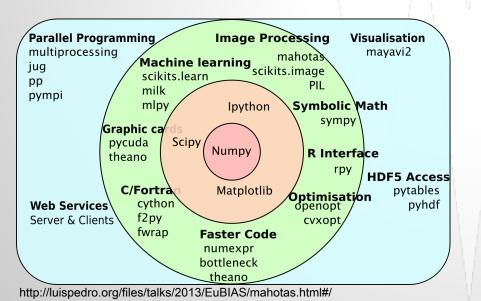
- Widely used in all areas, picking up lots of momentum in many sciences
- Simple, concise, and easy-to-read syntax
- Free and Open Source, <u>large scientific</u>
 <u>community</u>
 - ⇒ potentially high impact / user base
- general purpose programming language
- Cross-platform: from RaspberryPi to large supercomputers

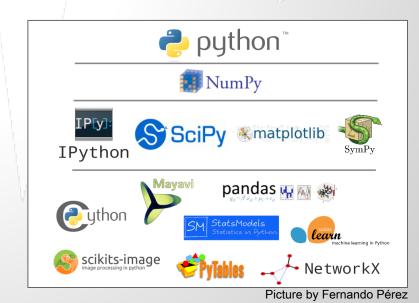




Why Python?

- No need to compile, <u>interactive shell available</u>
- Easy to <u>interact with existing C and Fortran</u>
 code
- Vast scientific ecosystem; taking advantage of developments in other sciences





What is **ObsPy**?

Python library to work with seismological data

- waveform data
- station metadata
- event metadata

Facilitates development

- from short code snippets
- to complex processing workflows

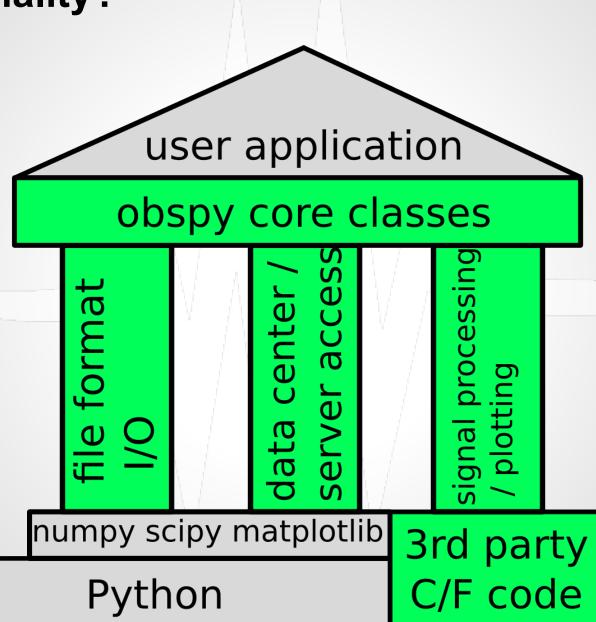
Develop once, use everywhere

=> a bridge for seismologists into the scientific Python ecosystem

Processing needs

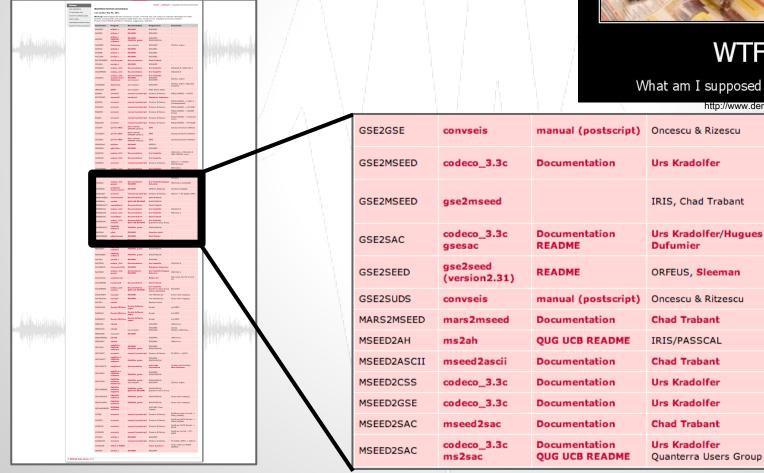
What I need is...

- .. I/O of local data
- .. fetch data/metadata from data centers
- .. convenient handling of the parsed data/metadata
- .. basic signal processing / data analysis / math
- .. visualization capabilities



File Formats

Situation before ObsPy





http://www.demotivation.us/search/all/wtf-1266995.html

UNIX HP/SUN, Linux

GSE1.0/2.x, SAC(A/B)

Handling metadata

CSS2.8/3.0

GSE1.0/2.x

GSE 2.x/IMS 1.0, INT or CM6

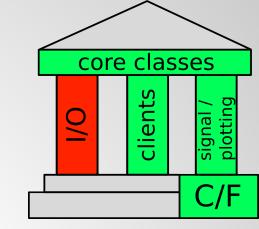
Solaris, Linux, Mac OSX and

GSE1.0 -> PC-SUDS (.DMX)

DOS/Windows GSE1.0/2.x

Windows

read/write support for lots of formats:



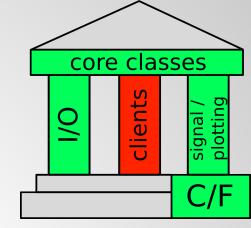
- waveforms (MiniSEED, GSE2, SAC, ...)
 - many different ways to store binary/encoded timeseries
- station metadata (SEED, <u>StationXML</u>)
 - complex, esp. instrument response
- event metadata (<u>QuakeML</u>, NDK, PDE)
 - complex associations, owed to how data is assembled in realtime systems

data center access (archived data):

- FDSN web service client
 - o IRIS, Orfeus, USGS, RESIF, NCEDC, ...
- ArcLink client: <u>EIDA</u> / Orfeus
- <u>SeisHub</u>: FFB, local database systems
- ...

server access (near-realtime / ringbuffer data):

- SeedLink, Earthworm
- ⇒ different types of servers, but usage of clients very similar

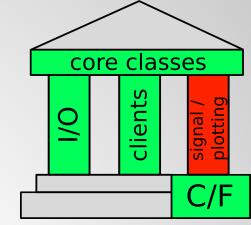


basic signal processing:

- trim, merge, rotate, ...
- filter, resample, instrument correction
- array analysis, cross correlations
- (coincidence) triggering (incl. master event detection)
- probabilistic power spectral densities

basic plotting:

- waveform preview plots
- stations/events location plots
- channel instrument response plots (bode plots)

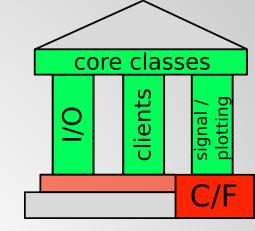


3rd party code:

- don't reinvent the wheel
- reuse well established and maintained code

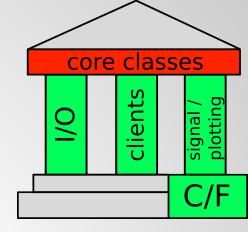
we use..

- <u>numpy</u>: fast array operations
- scipy: signal processing routines
- libmseed: MiniSEED I/O (IRIS)
- evalresp: instrument correction (<u>ISTI/IRIS</u>)
- iaspei-tau: theoretical traveltimes (Snoke etal.)
- GSE_UTI: GSE2 I/O (Stange etal.)

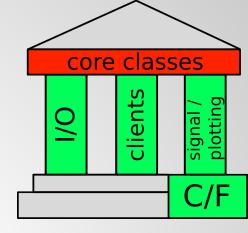


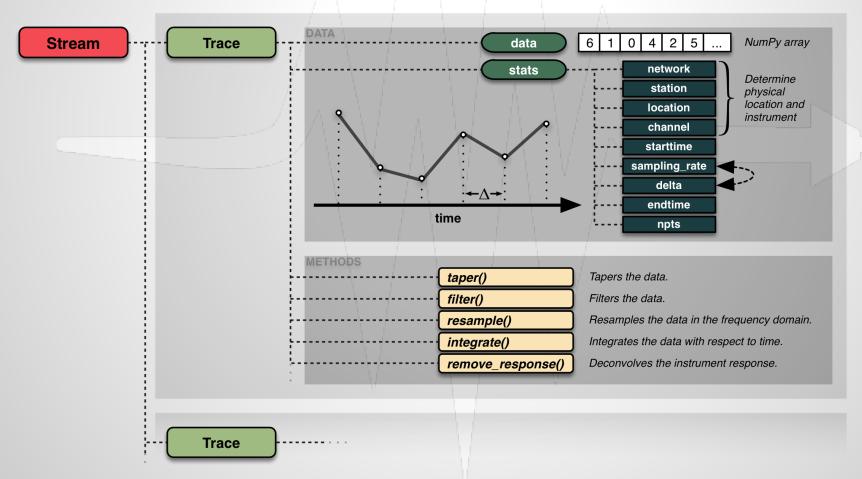
core object classes:

- waveforms
 - ⇒ Trace / Stream
- station metadata
 - ⇒ Inventory / Network / Station / ...
- event metadata
 - ⇒ Catalog / Event / ...

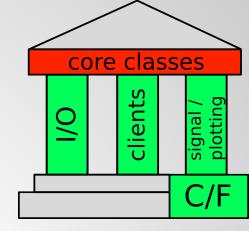


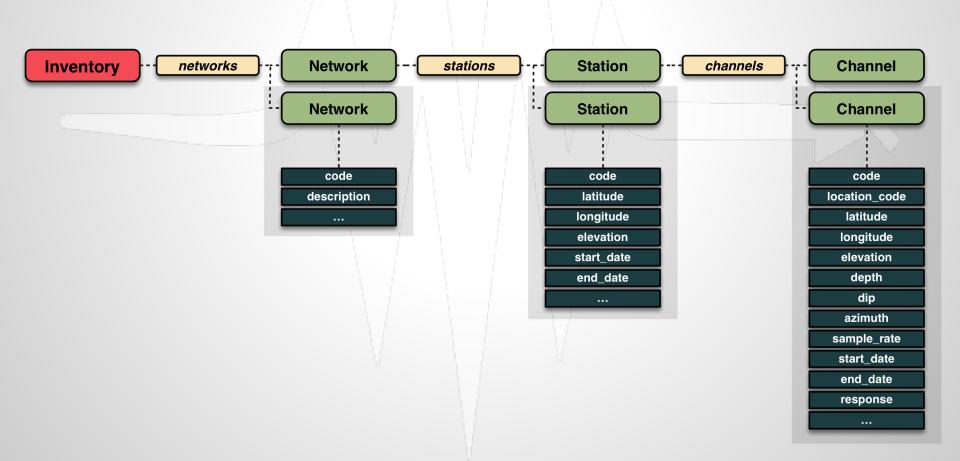
core object classes: waveforms



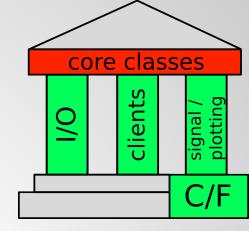


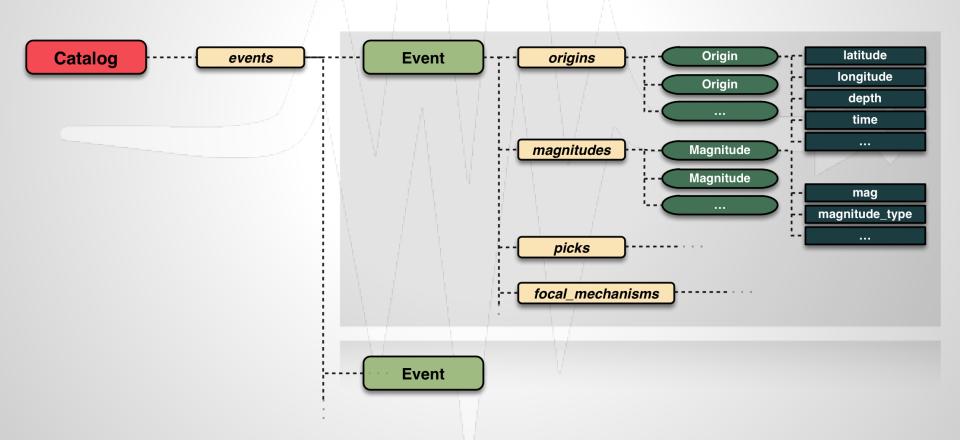
core object classes: station metadata

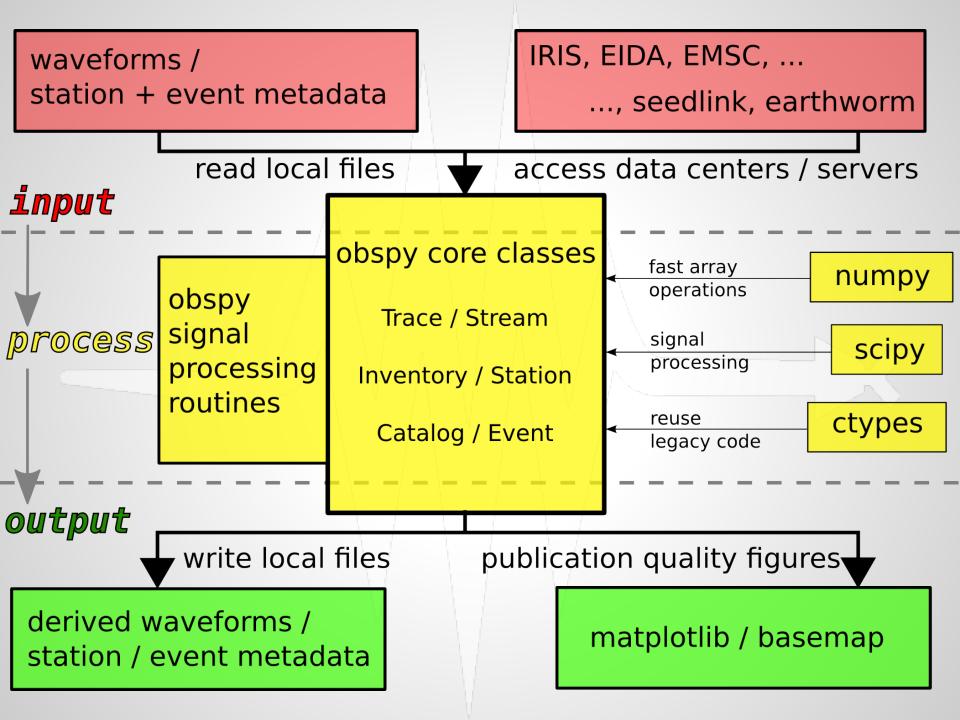




core object classes: event metadata







```
from obspy import read
In [2]:
            stream = read("waveform.mseed")
            stream.plot()
             2014-05-31T10:37:20Z - 2014-05-31T10:39:20Z
                                                               GR.FUR..BHZ
                 77074
                 51235
                 25397
                  -440
                -26278
                -52117
                -77955
                   10:37:20
                                                 10:38:00
                                                                               10:38:40
                                                                                                             10:39:20
                                                              GR.FUR..BHN
                 76860
                 51022
                 25183
                  -654
                -26492
                -52331
                -78169
                   10:37:20
                                                 10:38:00
                                                                               10:38:40
                                                                                                             10:39:20
```

10-3

10-2

10-1

10°

Frequency [Hz]

10¹

10²

```
from obspy import read inventory
In [3]:
         inventory = read inventory("station.xml")
         channel = inventory[0][0][0]
         print channel
         channel.plot(0.001)
         Channel 'HHZ', Location ''
                 Timerange: 2006-12-16T00:00:00.000000Z - --
                 Latitude: 48.16, Longitude: 11.28, Elevation: 565.0 m, Local Depth: 0.0 m
                 Azimuth: 0.00 degrees from north, clockwise
                 Dip: -90.00 degrees down from horizontal
                 Channel types: TRIGGERED, GEOPHYSICAL
                 Sampling Rate: 100.00 Hz
                 Sensor: Streckeisen STS-2/N seismometer
                 Response information available
                        0.02
            10°
                                                         9.4e+08
         Amplitude
            10<sup>8</sup>
            107
          Phase [rad]
```

```
In [4]:
            stream.attach_response(inventory)
            stream.remove_response(output="VEL")
            stream.plot()
             2014-05-31T10:37:20Z - 2014-05-31T10:39:20Z
                                                               GR.FUR..BHZ
                7.9e-05
                5.3e-05
                2.6e-05
                4.4e-08
               -2.6e-05
               -5.3e-05
               -7.9e-05
                   10:37:20
                                                  10:38:00
                                                                                10:38:40
                                                                                                              10:39:20
                                                               GR.FUR..BHN
                7.9e-05
                5.3e-05
                2.6e-05
                3.4e-08
               -2.6e-05
               -5.3e-05
               -7.9e-05
                   10:37:20
                                                  10:38:00
                                                                                10:38:40
                                                                                                              10:39:20
```

Technical Aspects

- Testing Framework
 - Testing code
 - Test reporting / Continuous Integration
- Version Control + Code Hosting
 - git: distributed version control
 - github: central platform for hosting, "social coding"

Technical Aspects: Testing? Why?

- correctness of code
- stability of code
- when you fix a bug you want to make sure it stays fixed
- everybody can work on the code even if he/she does not know all details of the implementation
- documentation

Technical Aspects: Doctests

```
class UTCDateTime(object):
    def __add__(self, value):
         Adds seconds and microseconds to current UTCDateTime object.
         :type value: int, float
         :param value: Seconds to add
         :rtype: :class:`~obspy.core.utcdatetime.UTCDateTime`
         :return: New UTCDateTime object.
         .. rubric:: Example
         >>> dt = UTCDateTime(1970, 1, 1, 0, 0)
         >>> dt + 1.123456
                                                                                         DOCUMENTATION
         UTCDateTime(1970, 1, 1, 0, 0, 1, 123456)
                                                        obspy.core.utcdatetime.UTCDateTime.__add_
         if isinstance(value, datetime.timedelta)
             value = (value microseconds + (value)
                                                        UTCDateTime. add (value)
                  86400) * 1000000) / 1000000.0
                                                        Adds seconds and microseconds to current UTCDateTime object.
         return UTCDateTime(self.timestamp + value)
                                                         Parameters: value (int, float) Seconds to add
                                                         Return type: UTCDateTime
if name == ' main ':
                                                         Returns:
                                                                New UTCDateTime object.
    import doctest
    doctest.testmod(exclude empty=True)
                                                        Example
                                                         >>> UTCDateTime(1970, 1, 1, 0, 0) + 1.123456
 SOURCE CODE
                                                         UTCDateTime(1970, 1, 1, 0, 0, 1, 123456)
```

Technical Aspects: Unit tests

```
from obspy.core import UTCDateTime
import unittest
class UTCDateTimeTestCase(unittest.TestCase):
    Test suite for obspy.core.utcdatetime.UTCDateTime.
    def test_weekday(self):
        Tests weekday method.
        dt = UTCDateTime(2008, 10, 1, 12, 30, 35, 45020)
        self.assertEquals(dt.weekday, 2)
    def test_invalidDates(self):
        Tests invalid dates.
        self.assertRaises(ValueError, UTCDateTime, 2010, 9, 31)
        self.assertRaises(ValueError, UTCDateTime, '2010-09-31')
def suite():
    return unittest.makeSuite(UTCDateTimeTestCase, 'test')
if name == ' main ':
    unittest.main(defaultTest='suite')
```

megies@wintermute: ~/git/obspy	×
megies@wintermute: ~/git/obspy/obspy/mseed	×
wintermute:~/git/obspy[<u>releases</u>]\$ obspy-runtests -r	
S	
Ran 983 tests in 103.554s	
ок	
Test report has been sent to tests.obspy.org. Thank you! wintermute:~/git/obspy [[] releases]\$	

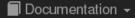
```
megies@wintermute: ~/git/obspy/obspy/mseed
                                                 megies@wintermute: ~/git/obspy/obspy/mseed
 megies@wintermute: ~/git/obspy
14
15 def getStartAndEndTime(file or file object):
16
17
        Returns the start- and endtime of a Mini-SEED file or file-like object.
18
19
20
21
22
        :return: tuple (start time of first record, end time of last record)
23
24
        This method will return the start time of the first record and the end time
25
           the last record. Keep in mind that it will not return the correct result
~/git/obspy/obspy/mseed/util.py [TYPE=PYTHON]
                                                                              15,5
        >>> f.close()
70
71
72
        # Get the starttime of the first record.
73
        info = getRecordInformation(file or file object)
        starttime = info['starttime']
74
75
        # Get the endtime of the last record.
76
        info = getRecordInformation(
77
            file or file object,
78
            (info['number of records'] - 1) * info['record length'])
        endtime = info['endtime']
79
80
        return starttime, endtime
~/git/obspy/obspy/mseed/util.py
                                   [TYPE=PYTHON]
                                                                              78,39
                                                                                              10%
```

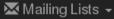
```
megies@wintermute: ~/git/obspy
 megies@wintermute: ~/git/obspy
                                             megies@wintermute: ~/git/obspy/obspy/mseed
File "/home/megies/git/obspy/obspy/mseed/util.py", line 67, in obspy.mseed.util.getStartAnd
EndTime
Failed example:
    getStartAndEndTime(file object) # doctest: +NORMALIZE WHITESPACE
Exception raised:
    Traceback (most recent call last):
      File "/home/megies/python276/lib/python2.7/doctest.py", line 1289, in run
        compileflags, 1) in test.globs
      File "<doctest obspy.mseed.util.getStartAndEndTime[12]>", line 1, in <module>
        getStartAndEndTime(file object) # doctest: +NORMALIZE WHITESPACE
      File "/home/megies/git/obspy/obspy/mseed/util.py", line 73, in getStartAndEndTime
        info = getRecordInformation(file or file object)
      File "/home/megies/git/obspy/obspy/mseed/util.py", line 253, in getRecordInformation
        endian=endian)
      File "/home/megies/git/obspy/obspy/mseed/util.py", line 288, in getRecordInformation
        elif file object.read(8)[6] not in ['D', 'R', 'Q', 'M']:
    IndexError: string index out of range
Ran 983 tests in 100.804s
FAILED (failures=1, errors=1)
Test report has been sent to tests.obspy.org. Thank you!
wintermute:~/git/obspy[releases]$
```

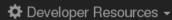




20 - records per page







show all ○ errors only

Search Docs

Test Reports Overview of the latest 20 test reports

records per page					o onow all o onor only		
Report	Errors / Failures	ObsPy Version	Tests	Modules	Node Name	Python Version	System
* #15439	1	0.9.2-805- gdbc825	1053	21	travis-ci	3.4.0	Linux (64bit)
* #15438	3	0.9.2-746- ga194a	1047	21	docker- debian_7_wheezy	2.7.3	Linux (64bit)
* #15437	3	0.9.2-746- ga194a	1047	21	docker-fedora_20	2.7.5	Linux (64bit)
# 15436	-	0.9.2-805- gdbc825	1053	21	travis-ci	3.3.5	Linux (64bit)
* #15435	26	0.9.2-787-gf176	1186	28	sphinx	2.7.3	Linux (32bit)

System

- all
- Darwin
- Linux
- Windows

Architecture

- all
- 32bit
- 64bit

Python

- all
- 2.6.0
- 2.6.1
- 2.6.5
- 2.6.62.6.7

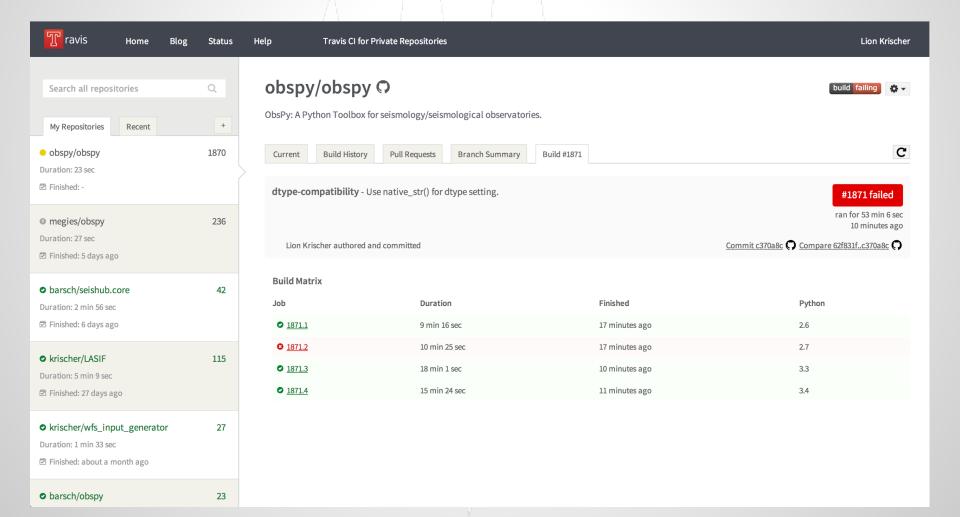
Technical Aspects: Testing

Continuous Integration

- automate the build (incl. dependencies)
- automate running all tests
- trigger building/testing automatically on changes in the repository
- online overview of build/test results
- keep building/testing fast
- each pull request is automatically tested

Technical Aspects: Testing

Travis: free CI service for open source projects



Technical Aspects: GitHub





GitHub: Free hosting of code repositories

- De facto standard for code hosting
- Worldwide community of developers
- Issue / bug tracker
 (add comments, commits, integration with Travis CI)
- Social coding and communication
- Forking, pull requests
- Avoids overhead of self-hosting
- Visibility
- New: <u>DOIs for Code</u> => citable

Technical Aspects: git

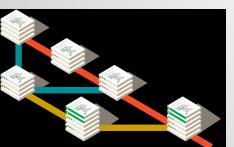


git: distributed version control software

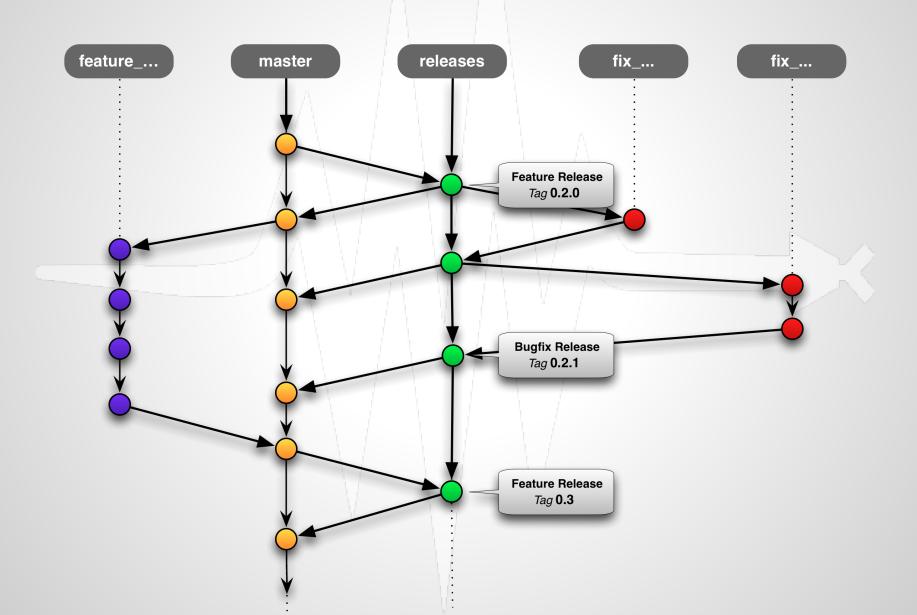
- Initialized 2005 by Linus Torvalds for managing the Linux kernel
- Every local copy of the repository is selfcontained with full history
- Possible to work offline
- Strong support for branching / merging

"Subversion used to say 'CVS done right' [...] There is no way to do CVS right."

Linus Torvalds



Technical Aspects: ObsPy Dev Model



Spreading the word: why?

start of the project ...

.. group of a few dedicated (under)grad students

but ..

- .. people go different ways
- .. and unmaintained projects die fast

ultimate goal: self-sustaining project

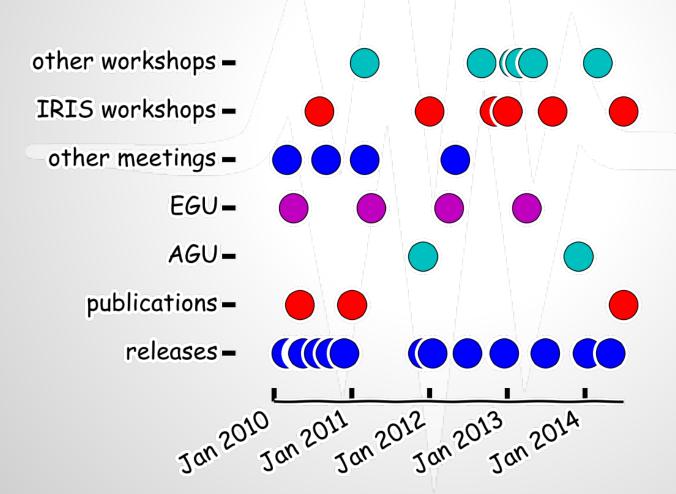
- .. get more contributors/developers/maintainers
- .. raise impact
- .. reach critical mass of users / institutions relying (depending?) on the project

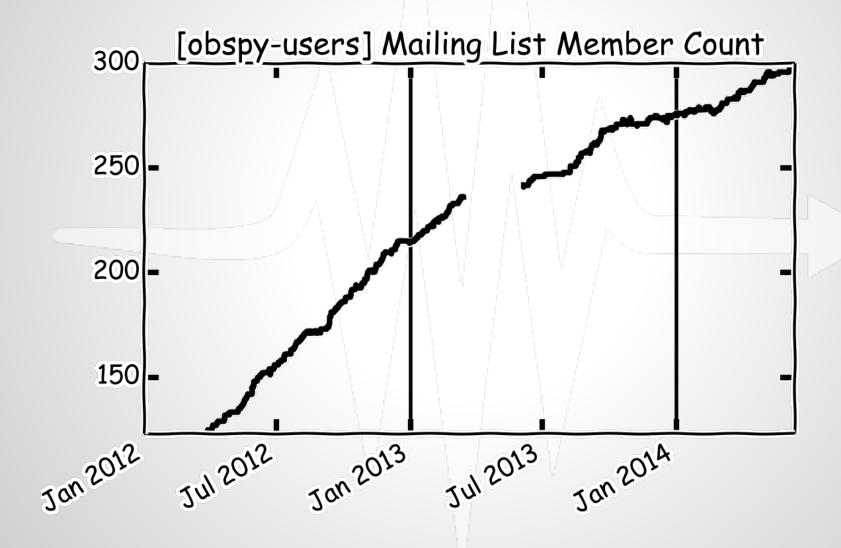
Spreading the word: homework...

- make it ..
 - .. useful
 - .. easy to use
 - good <u>documentation</u>
 - tutorial, gallery, workshop documents online
 - .. easy to install (on any platform)
 - available at pypi
 - binaries, installers, packages
 - .. reliable (tests!)
 - .. interactive and responsive
 - o github, wiki, mailing list

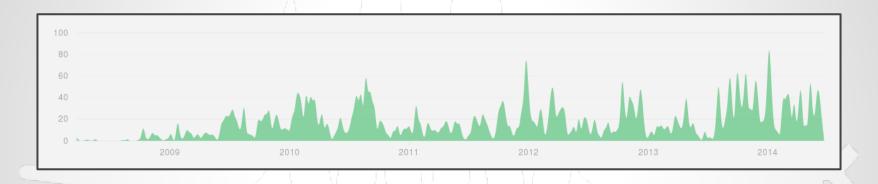
Spreading the word: how?

..wherever we go, we tell people about it



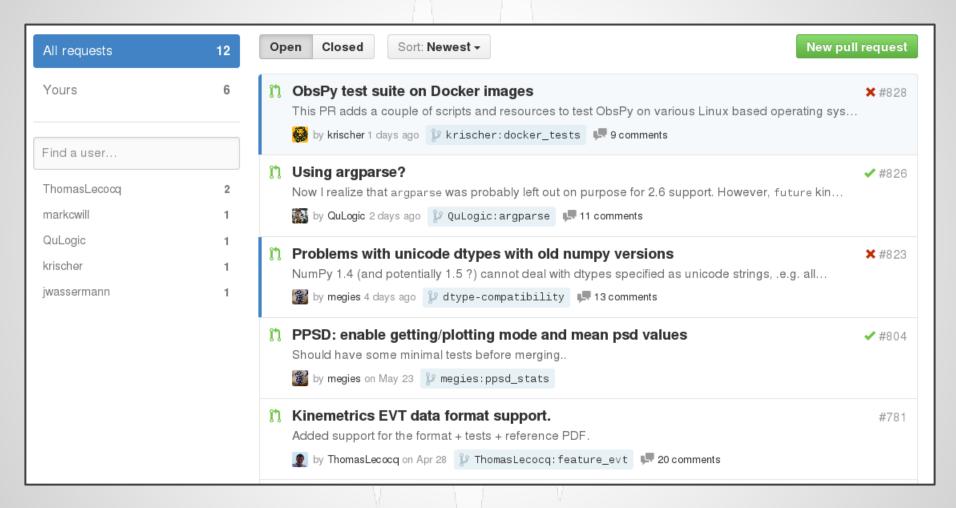


some stats...



- 30 people have actively committed changesets on github
- ~ 10 people sent contributions as Python files via email

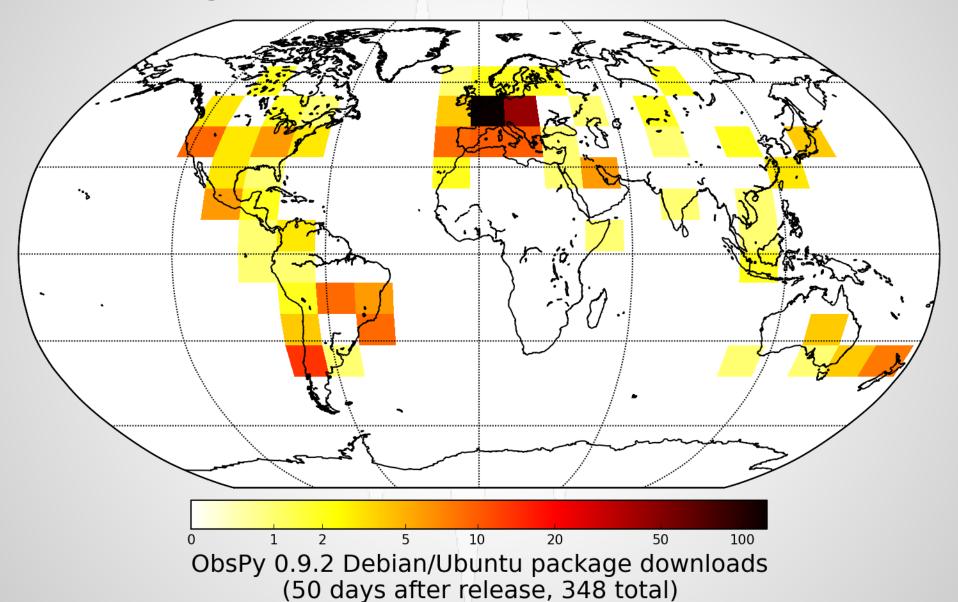
<u>59 citations</u> of our <u>publications</u>



lot of <u>active discussions</u> about improvements

growing number of contributions from "outside"

- clients (3/9): seedlink, earthworm, neic
- file format plugins: css, datamark, pde, y
- packaging efforts:
 - Fedora / RHEL / CentOS
 - ArchLinux
 - FreeBSD
 - NetBSD
 - MacPorts



Summary

ObsPy

..addresses most needs for successful and fast development of custom processing

..being reproducible

..and easing up exchange of processing workflows

..it is widely known, used and acknowledged

..and has grown from a 2-4 man show to being developed by people from all around the world



Thanks for your attention!

www.obspy.org