Argonne NATIONAL LABORATORY

ARM CLIMATE RESEARCH FACILITY

The Language, Libraries and Culture of Python in Meteorology

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python™

NumPy

Cython

SciPy

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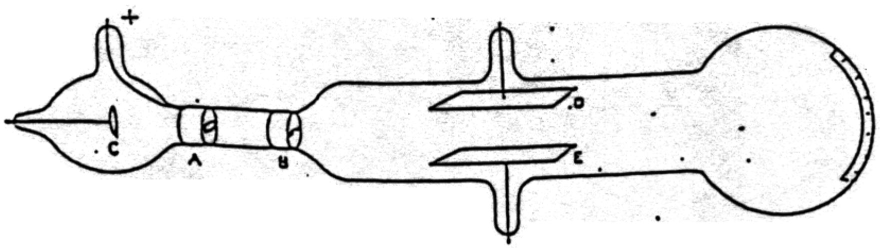
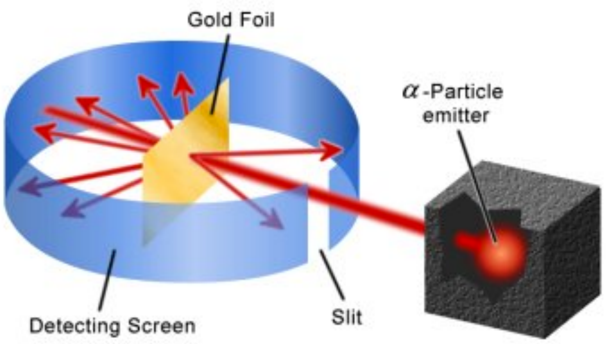
U.S. DEPARTMENT OF ENERGY

Technology Powers Scientific Discovery

- Scientific advancements are driven by state-of-the-art technologies.
- New technologies lead the way to scientific breakthroughs and a more complete understanding of the world around us.

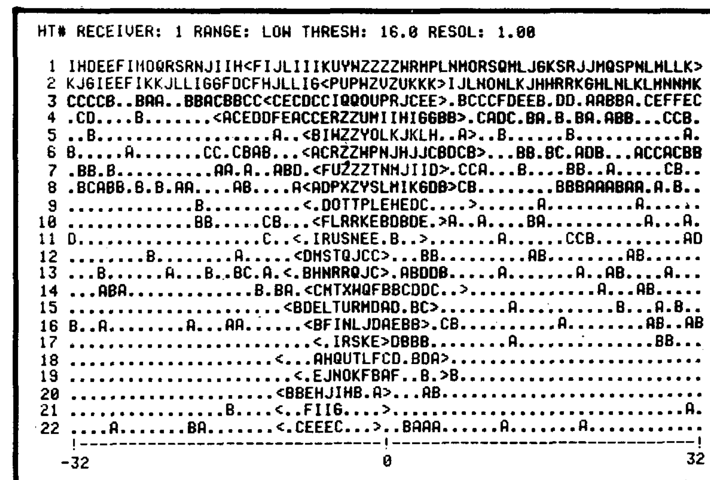




Computers Prime Technology for Science

- Computers are the most significant technology available to scientists today.
- The ability to perform fast computations has vastly changed meteorology and will continue to change the field in the future.

ARM CSAPR Radar
http://www.arm.gov/instruments/csapr



```
HT# RECEIVER: 1 RANGE: LOW THRESH: 16.0 RESOL: 1.00

 1 IHDEEFIMOQRSRNJIIH<FIJLIIIKUYWZZZZWRMPLNMORSQMLJGKSRJJMQSPNLMLLK>
 2 KJGIEEFIKKJLLIGGFDCFHJLLIG<PUPWZVZUKKK>IJLNONLKJHHRRKGHLNLKLHNNMK
 3 CCCCB..BAA..BBACBBCC<CECDCCIQQOUPRJCEE>.BCCCFDEEB.DD.AABBA.CEFFEC
 4 .CD....B.......<ACEDDFEACCERZZUMIIHIGGBB>.CADC.BA.B.BA.ABB...CCB.
 5 ..B..................A..<BIHZZYOLKJKLH..A>..B......B...........A.
 6 B.....A.......CC.CBAB...<ACRZZHPNJHJJCBDCB>...BB.BC.ADB...ACCACBB
 7 .BB.B..........AA.A..ABD.<FUZZZTNMJIID>.CCA...B....BB..A.....CB..
 8 .BCABB.B.B.AA....AB....A<ADPXZYSLMIKGDB>CB........BBBAAABAA.A.B..
 9 ..............B..........<.DOTTPLEHEDC....>......A..........A.....
10 ..............BB.....CB...<FLRRKEBDBDE.>A..A....BA...........A...A.
11 D...................C..<.IRUSNEE.B..>.......A......CCB.........AD
12 .........B.........A.....<DMSTQJCC>...BB..........AB.........AB......
13 ...B......A...B..BC.A.<.BHNRRQJC>.ABDDB.....A........A..AB....A...
14 ...ABA..............B.BA.<CMTXWQFBBCDDC..>..............A...AB.....
15 .....................<BDELTURMDAD.BC>.......A...........B...A.B..
16 B..A.........A...AA.......<BFINLJDAEBB>.CB...........A.........AB..AB
17 .........................<.IRSKE>DBBB.........A..................BB...
18 ......................<...AHQUTLFCD.BDA>............................
19 .......................<.EJNOKFBAF..B.>B.........................
20 ......................<BBEHJIHB.A>...AB..........................
21 ................B....<..FIIG....>...............................A.
22 ....A........BA.......<.CEEEC...>..BAAA......A........A............
   !------------------------------!------------------------------!
  -32                             0                              32
```

FIG. 7. Sample of real-time Doppler spectra available to a radar operator by telephone.

Source: R. G. Strauch *el al*, JTech, **1984**, 1, 37

Programming: Controlling Computers for Science

- The daily operation of science involves computers.
- Computers require specific directions in the form of software to realize their potential to power scientific research and operations.
- The ability to create software customized to a specific scientific task is often needed.
- Writing software can be a time consuming and burdensome task.
  - Scientists estimate that 35% of their research time is spent developing software [1].
  - Most scientists learn to develop software informally from their peers [2].
  - The choice of programming language affects the time required for development.

[1] P. Prabhu, et al, A Survey of the Practice of Computational Science, **2011**, 10.1145/2063348.2063374
[2] J. E. Hannay, *et al*, How Do Scientists Develop and Use Scientific Software, **2009**, 10.1109/SECSE.2009.5069155.

Python is Ideal for Writing Scientific Software

- Python is the ideal programming language for writing software to meet the computational challenges in meteorology and atmospheric science.

- Developing software in Python is simple and fast due to:
  - The design and philosophy of the **language**.
  - The availability of a number of high-quality, efficient scientific Python **libraries.**
  - The welcoming, vibrant, and growing Python **community**.

Python: the Language

Python, the programming language is:

- A **high-level** language.
  - Allows one to focus on the the task concepts rather than the details of the computer.
  - Makes development simple and quick.

- **Interpreted** and interactive.
  - No compilation step, speeds up development cycle.
  - Interactive shell (REPL) for testing and debugging.

- **General purpose**.
  - Can be used to write software across a wide range of applications, not domain specific.
  - Larger user and developer base.

Python: the Language

Python is an ideal language for scientific programming because it is:

- **Concise** and **readable**

Python

```python
colors = ['red', 'blue', 'green']
for color in colors:
    print(color)
```

Perl

```perl
@colors = ("red", "blue", "green");
foreach (@colors) {
    print "$_\n”;
}
```

- **Open Source** and **Free**
  - No company controls the software, no licensing costs.

- Has a large number of third-party **libraries**.
  - PyPI contains more than 72,000 packages.
  - Many science-focused libraries exist covering a variety of fields.

- Easy to **interface** with existing C, C++ and Fortran code.
  - Tools like Cython, cffi, ctypes, and F2PY make interfacing with existing code simple.

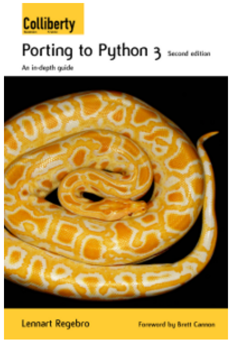
Python: the Challenges

Python does face some challenges:

- Execution speed is **slow** compared to some programming languages.
  - Many tasks are not limited by execution speed.
  - Options exist to speed up Python code.

- The language is not the best at some types of **parallel** computations.
  - The Global Interpreter Lock (GIL) poses limits of multi-threaded performance.
  - Handling concurrency is not as robust as some languages (Go, Erlang, Clojure).
  - Support for computation on GPUs and other highly parallel architectures is limited and requires additional libraries (Numba, PyCUDA)

- The language is currently **in flux**.
  - Python 3 is backwards incompatible with Python 2.
  - Some libraries do not support Python 3.



Scientific Python Libraries: Introduction

The Scientific Python Ecosystem or **SciPy stack** is a collection of open source software for scientific computing in Python. Some of the core packages are:

- **NumPy** : Provides powerful, efficient multi-dimensional arrays in Python
- **SciPy** : Fundamental numerical algorithms for common tasks in science.
- **matplotlib** : comprehensive publication-quality 2D plotting

- **Jupyter/IPython** : Rich, interactive interfaces for processing data and testing ideas.
- **pandas** : High performance, easy to use data structures.
- **SymPy** : Symbolic mathematics and computer algebra

The Python ARM Radar Toolkit: Py-ART

- Py-ART is a module for visualizing, correcting and analyzing **weather radar data** using packages from the scientific Python stack.
- Development began to address the needs of the **ARM** program with the acquisition of **multiple scanning cloud and precipitation radars**.
- The project has since been expanded to work with a **variety of weather radars**, including NEXRAD, and has a wide user base including radar researchers, weather enthusiasts and climate modelers.
- Available on GitHub as **open source software**, arm-doe.github.io/pyart/.
- Conda packages are available at anaconda.org/jjhelmus

ANACONDA CLOUD

Scientific Python Libraries: NumPy

- NumPy is the fundamental package for scientific computation in Python.

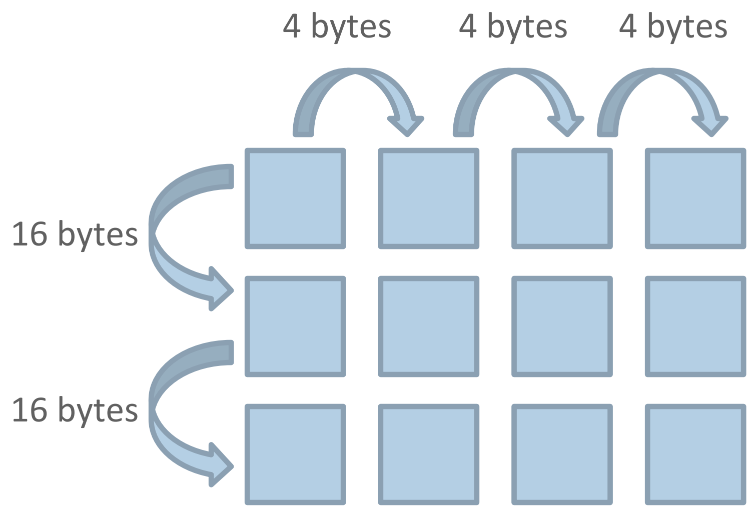
- NumPy provides:
  - Powerful, efficient (fast) multi-dimensional **array object**, the ndarray class.
  - Robust methods for **manipulating** these arrays.
  - Masked and record array objects.
  - Routines for linear algebra, Fourier transform, and random numbers.
  - Comprehensive, well-written documentation, http://docs.scipy.org/doc/.

- Other scientific Python packages build on NumPy to add additional features and abilities.

NumPy’s ndarray details

- NumPy’s core functionality is provided by its **ndarray** object.
- A ndarray is a **homogeneous**, **strided** view on a **contiguous** block of memory.

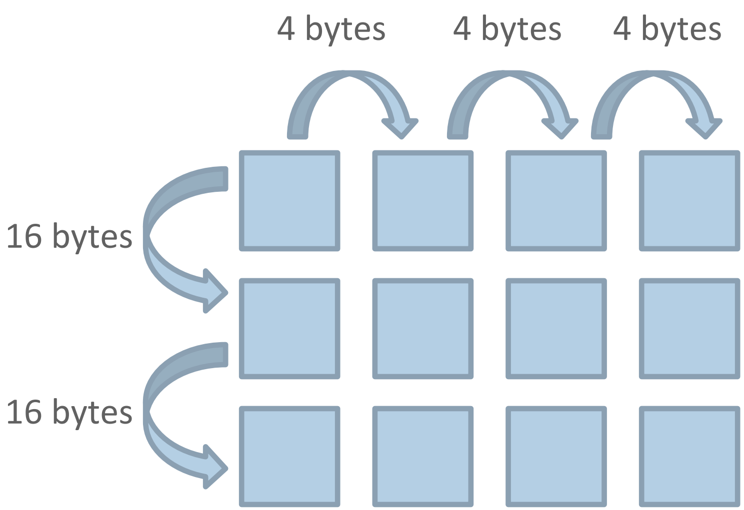
(3, 4) ndarray of float32
strides (16, 4)



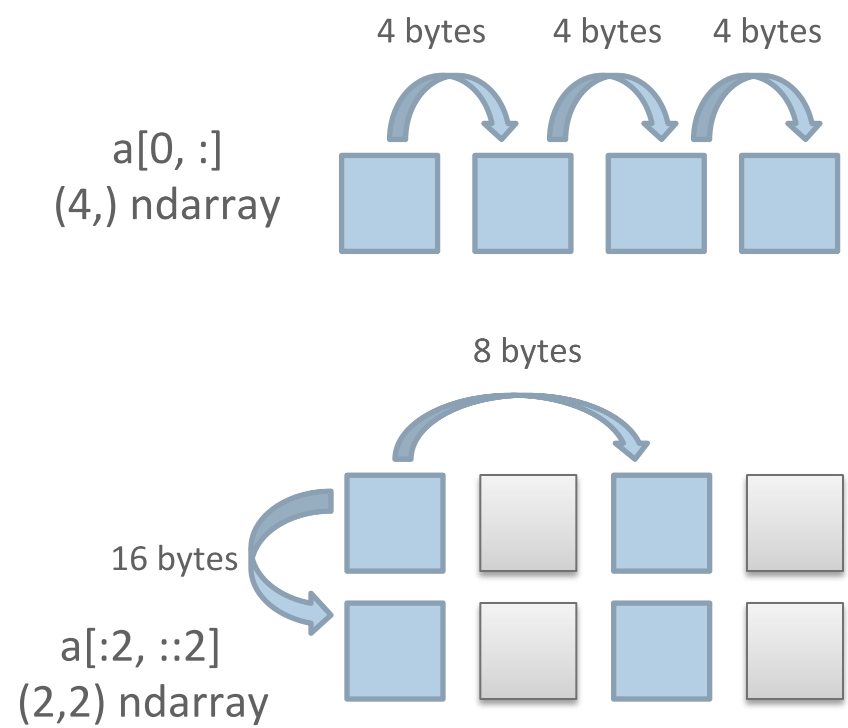
- Although simple, the ndarray is a **powerful construct** as the location of underlying memory can be passed to other languages (C, C++, Cython and Fortran) without the need to copy data.

ndarray views

- Slicing a NumPy ndarray almost always creates a “**view**” of the data.



a = np.zeros((3, 4), np.float32)
(3,4) ndarray



- No copying of data is needed when accessing or modifying views.

NumPy in Py-ART

NumPy is used extensively throughout Py-ART as ndarrays are the primary objects used to store and manipulate numerical data.

```
elif data_type_name == 'PHIDP2':
    out[:] = 360. * (data.view('uint16') - 1.) / 65534.
    mask[data.view('uint16') == 0] = True

elif data_type_name == 'HCLASS2':
    out[:] = data.view('uint16')

elif data_type_name == 'XHDR':
    # Here we return an array with the times in milliseconds.
    return data[..., :2].copy().view('i4')

# one byte data types
elif data_type_name[-1] != '2':
    # make a view of left half of the data as uint8,
    # this is the actual ray data collected, the right half is blank.
    nrays, nbin = data.shape
    ndata = data.view('(2,) uint8').reshape(nrays, -1)[:, :nbin]
```

NumPy in Py-ART

```
# decode run length encoding
rle_size = radial_header['nbytes'] * 2
rle = np.fromstring(buf2[pos:pos+rle_size], dtype='>u1')
colors = np.bitwise_and(rle, 0b00001111)
runs = np.bitwise_and(rle, 0b11110000) // 16
radial[:] = np.repeat(colors, runs)
```

Scientific Python Libraries: SciPy

SciPy is a collection of mathematical algorithms and functions which build upon NumPy to provide efficient solutions to common numerical tasks.

SciPy is divided into subpackages which cover a number of scientific domains:

- Image processing
- Signal processing
- Interpolation
- Spatial data structures and algorithms
- Clustering
- Numerical integration
- Differential equations
- Statistics
- Sparse matrices

SciPy in Py-ART

SciPy functions for image processing, numerical integration, interpolation, spatial analysis and sparse matrix storage are all used in Py-ART.

```
import scipy.ndimage
…

def _find_regions(vel, gfilter, limits):
    """Find regions of similar velocity. """
    mask = ~gfilter
    label = np.zeros(vel.shape, dtype=np.int32)
    nfeatures = 0
    for lmin, lmax in zip(limits[:-1], limits[1:]):

        # find connected regions within the limits
        inp = (lmin <= vel) & (vel < lmax) & mask
        limit_label, limit_nfeatures = scipy.ndimage.label(inp)

        # add these regions to the global regions
        limit_label[np.nonzero(limit_label)] += nfeatures
        label += limit_label
        nfeatures += limit_nfeatures

    return label, nfeatures
```

Scientific Python Libraries: matplotlib

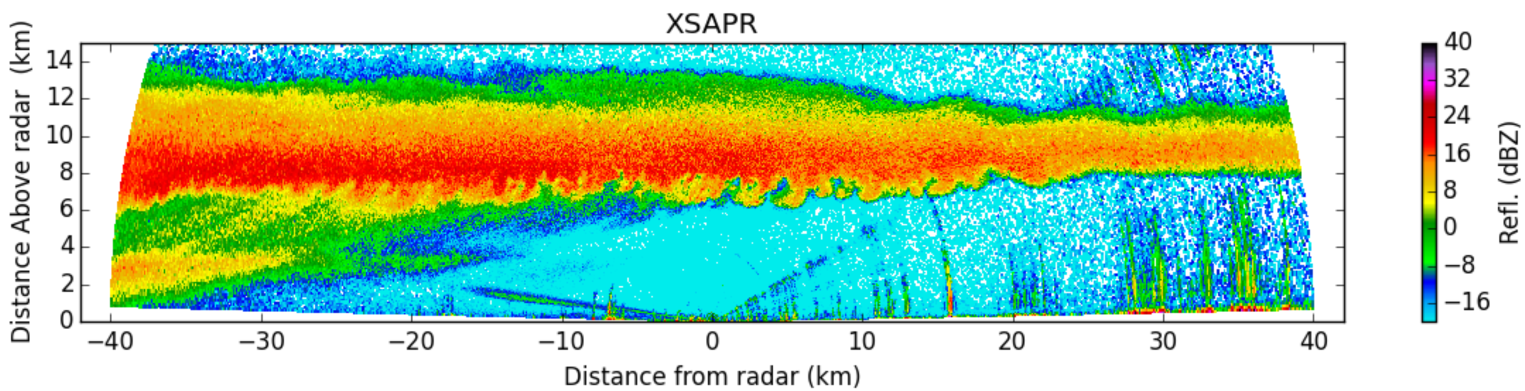
matplotlib is a plotting library which works with NumPy.

- Comprehensive 2D, publication quality plots.
  - Multiple plot types: line, scatter, image, contours, pseudocolor, …
  - Many output formats: png, jpg, svg, ps, pdf, …

- A limited set of 3D plots.
  - Line, scatter, wireframe, tri-surface, contour, polygon, …

- Plots can be examined interactively or embedded in applications.
  - Explore data in a GUI
  - ARTView : GUI viewer built on top of the Py-ART which embeds matplotlib plots

matplotlib in Py-ART



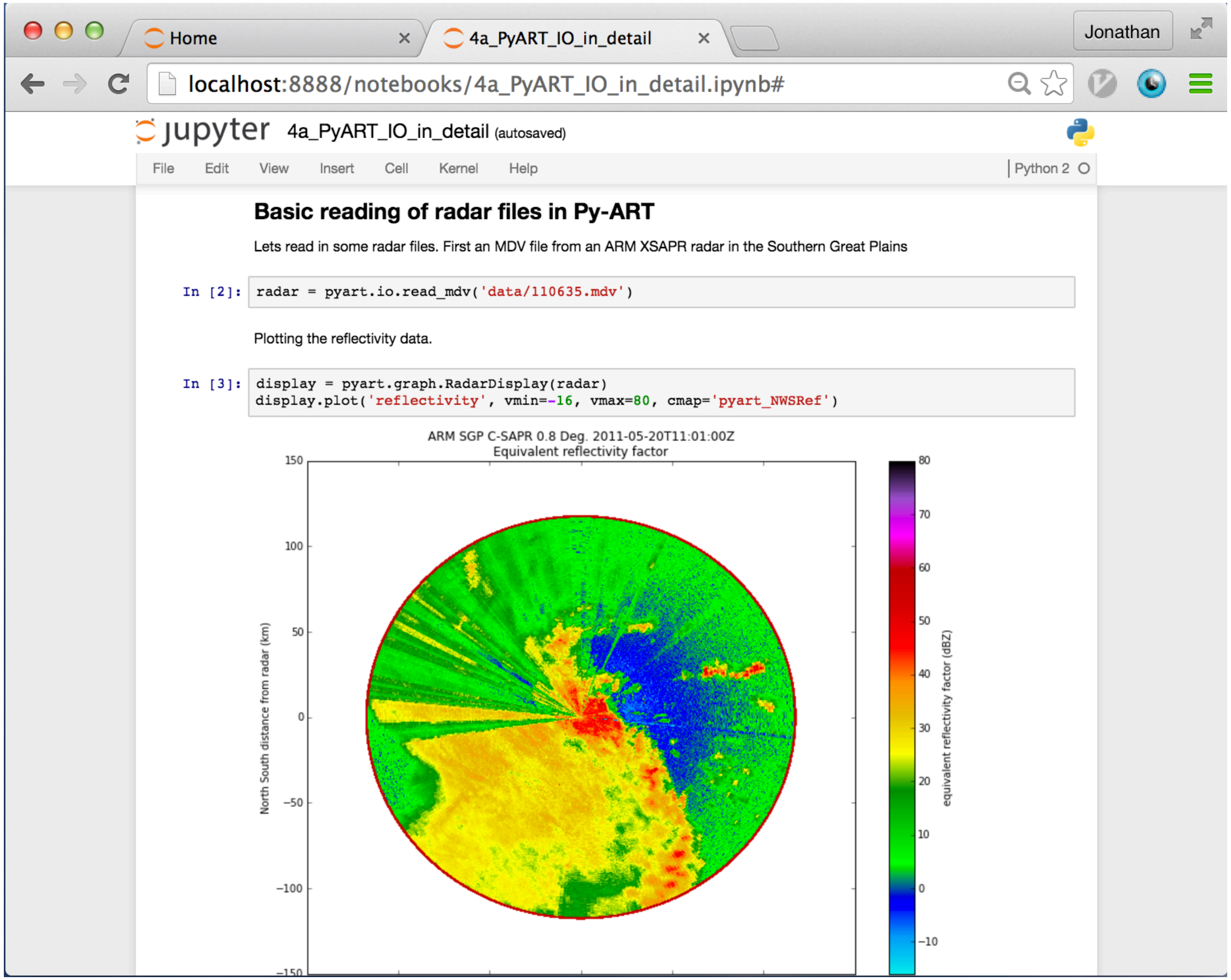

```
import matplotlib.pyplot as plt
import pyart

radar = pyart.io.read('sgpxsaprrhicmacI5.c0.20110524.015604_NC4.nc')
fig = plt.figure(figsize=(12, 3))

display = pyart.graph.RadarDisplay(radar)
display.plot('reflectivity_horizontal', vmin=-20, vmax=40,
             cmap='pyart_NWSRef', title='XSAPR', colorbar_label='Refl. (dBZ)')
display.set_limits(ylim=(0, 15), xlim=(-42, 42))

plt.tight_layout()
plt.savefig('figure.png')
```

Scientific Python Libraries: Jupyter/IPython

Project Jupyter (previously IPython) is a set of rich, interactive interfaces and tools for processing data and testing ideas in Python.

- User Interfaces
  - Juypter Console: Terminal based interactive Python environment
  - Juypter Notebook: Web based platform for authoring rich documents
  - Both have excellent integration with matplotlib
- Kernels
  - IPython: interactive computing in Python
  - ipyparallel: Lightweight parallel computing with notebook integration
  - IJulia, IRKernel, IRuby, IPerl, …
- Many other interesting tools: nbviewer, nbconvert, nbgrader, jupyterhub…

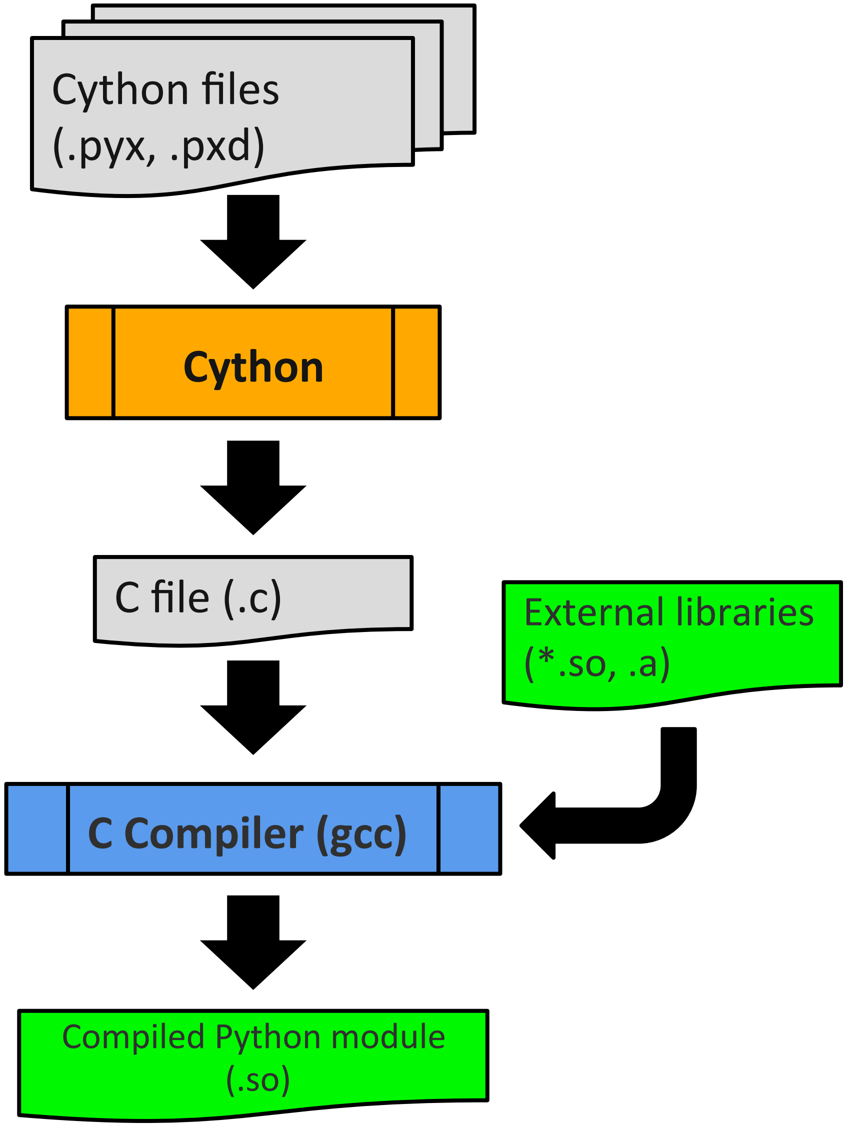
Jupyter/IPython in Py-ART



Scientific Python Libraries: Cython

Cython

- Python to C code translator.
- Generates a Python extension module.
- Can be used to speed up Python code by adding static type information.
- Also can be used to interact with C/C++ function and classes in external libraries.



Cython in Py-ART: wrapping libraries

_rsl_h.pxd

```
cdef extern from "rsl.h":

        ctypedef struct Radar:
            Radar_header h
            Volume **v

        ctypedef struct Radar_header:
            int month, day, year
            int hour, minute
            float sec
            ...

        ctypedef struct Volume:
            Volume_header h
            Sweep **sweep
            ...
    ...

    Radar * RSL_anyformat_to_radar(char *infile)
        ...
    void RSL_free_volume(Volume *v)
        void RSL_free_radar(Radar *r)
```

_rsl_interface.pyx

```
cimport _rsl_h

cdef class RslFile:
        cdef _rsl_h.Radar * _Radar
        cdef _rsl_h.Volume * _Volume

        def __cinit__(self, filename):
            self._Radar = _rsl_h.RSL_anyformat_to_radar(filename)
            if self._Radar is NULL:
                raise IOError('file cannot be read.')

        def __dealloc__(self):
            _rsl_h.RSL_free_radar(self._Radar)

        def get_volume(self, int volume_number):
            rslvolume = _RslVolume()
            rslvolume.load(self._Radar.v[volume_number])
            return rslvolume
        ...
        property month:
            def __get__(self):
                return self._Radar.h.month
            def __set__(self, int month):
                self._Radar.h.month = month
```

Cython in Py-ART: speeding up Python code

Cython

```
@cython.boundscheck(False)
@cython.wraparound(False)
def _fast_edge_finder(int[:, ::1] labels, float[:, ::1] data, int rays_wrap_around,
                      int max_gap_x, int max_gap_y, int total_nodes):
    """ Return the gate indices and velocities of all edges between regions. """
    cdef int x_index, y_index, right, bottom, y_check, x_check
    cdef int label, neighbor
    cdef float vel, nvel

    collector = _EdgeCollector(total_nodes)
    right = labels.shape[0] - 1
    bottom = labels.shape[1] - 1

    for x_index in range(labels.shape[0]):
        for y_index in range(labels.shape[1]):
            label = labels[x_index, y_index]
            if label == 0:
                continue
            vel = data[x_index, y_index]

            # left
            x_check = x_index - 1
            if x_check == -1 and rays_wrap_around:
                x_check = right     # wrap around
            if x_check != -1:
                neighbor = labels[x_check, y_index]
                nvel = data[x_check, y_index]
                ...
                # add the edge to the collection (if valid)
                collector.add_edge(label, neighbor, vel, nvel)
```

107 seconds vs. 0.234 seconds, x450 performance improvement.

More Scientific Python Libraries…

- pandas : data structures and analysis
- xray : labeled array and datasets
- Iris : meteorology/climate data model

- basemap : plot 2D data on maps
- pyproj : cartographic transformations
- Cartopy : cartographic tools for Python

- netCDF4-python : Read and write NetCDF files.
- h5py : Read and write HDF5 files

- scikit-learn : machine learning
- scikit-image : image processing

- And many, many more…

Python Community: Online

The Python **community** provides a welcoming, vibrant and helpful culture. Much of the community interactions occur online:

- **Websites**
  - Python.org: Documentation, tutorial, PyPI and a wiki.
  - Other websites, scipy.org, pyaos.johnny-lin.com
- **Social media**
  - Facebook, Twitter, Google+, IRC, YouTube
  - Blogs: planetpython.org and planet.scipy.org.
  - Podcasts: Talk Python to me and podcast.__init__
- **Mailing lists**
  - Nearly all the SciPy stack packages have their own mailing lists
  - PyAOS mailing list (pyaos.johnny-lin.com)

Python Community: in Person

The Python community also meets in person.

- Conferences
  - SciPy
  - PyCon
  - Local and specialized conferences (PyData, AMS)
  - Conference talks often available at pyvideo.org
- Local user groups
  - wiki.python.org/moin/LocalUserGroups
- Meetups and hackathons.
  - python.meetup.com

Python Community: for Developers

- Mailing lists
  - Many projects have a –dev mailing list
- Social coding sites
  - GitHub
  - Bitbucket
- NumFocus
- Scientific Python focused companies
  - Continuum Analytics
  - Enthought

My Own Path Through the Python Community

- Undergraduate - Chemistry at Michigan Technological University
- Ph.D. at The Ohio State University - Chemical Physics.
  - Learned to program in Python
  - Wrote nmrglue, a library for working with NMR data in Python
- Post-doc at UConn Heath Center
  - Continued to program in Python – signal processing for NMR
  - Attended first SciPy conference
- Advanced Algorithms Engineer at Argonne National Laboratory
  - Development lead of the widely used open source Py-ART project.
  - Contributing to other libraries in the SciPy stack.
  - Attend and at times present at SciPy, PyCon, ChiPy, …

Careers in Meteorology with Python Programming

Do you enjoy programming? Solving problems? Python?

- High Performance Computing (HPC)
- Information Processing Technologies
- Instrumentation and processing
- Data Assimilation
- Numerical Weather Prediction
- Climate and atmospheric modeling

Regardless of the career path you choose, learning Python will enhance your potential.

Questions?

Resources for Learning Python

- Websites
  - Python.org tutorial
  - Scipy Lecture Notes, www.scipy-lectures.org
- Books
  - "Think Python: How to Think Like a Computer Scientist" by Allen B. Downey
  - "Effective Computation in Physics: Field Guide to Research with Python" by Anthony Scopatz, Kathryn D. Huff
- In person
  - Tutorials at conference (PyCon, SciPy, AMS)
  - Software Carpentry, software-carpentry.org
- Videos
  - Many Python conferences makes their tutorials available on YouTube or pyvideo.org