The Language, Libraries and Culture of Python in Meteorology

Jonathan Helmus
Argonne National Laboratory, USA
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/capr

Source: R. G. Strauch et 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.

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

- **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.
  - 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

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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.

- 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.

- 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

a[0, :]  # (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.

```python
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]
```
# 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.

```python
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
```
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

```python
import matplotlib.pyplot as plt
import pyart

radar = pyart.io.read('sgpxsaprhrhicmacI5.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**
  - Jupyter Console: Terminal based interactive Python environment
  - Jupyter 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...
Basic reading of radar files in Py-ART

Let's read in some radar files. First an MDV file from an ARM XSNPR radar in the Southern Great Plains.

```python
In [2]: radar = pyart.io.read_mdv('data/110635.mdv')
```

Plotting the reflectivity data.

```python
In [3]: display = pyart.graph.RadarDisplay(radar)
display.plot('reflectivity', vmin=-16, vmax=80, cmap='pyart_NWSRef')
```

![Radar Reflectivity Plot](image)
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":

```c
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
```

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Cython in Py-ART: speeding up Python code

```python
@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.

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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...

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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
  - 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](http://pyvideo.org)

- **Local user groups**
  - [wiki.python.org/moin/LocalUserGroups](http://wiki.python.org/moin/LocalUserGroups)

- **Meetups and hackathons.**
  - [python.meetup.com](http://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, ...

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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](http://www.scipy-lectures.org)

- **Books**
  - “Think Python: How to Think Like a Computer Scientist” by Allen B. Downey

- **In person**
  - Tutorials at conference (PyCon, SciPy, AMS)
  - Software Carpentry, [software-carpentry.org](http://software-carpentry.org)

- **Videos**
  - Many Python conferences makes their tutorials available on YouTube or [pyvideo.org](http://pyvideo.org)