



Scientific Programming with the SciPy Stack

Shaun Walbridge

Kevin Butler



<https://github.com/scw/scipy-devsummit-2017-talk>

[High Quality PDF \(5MB\)](#)

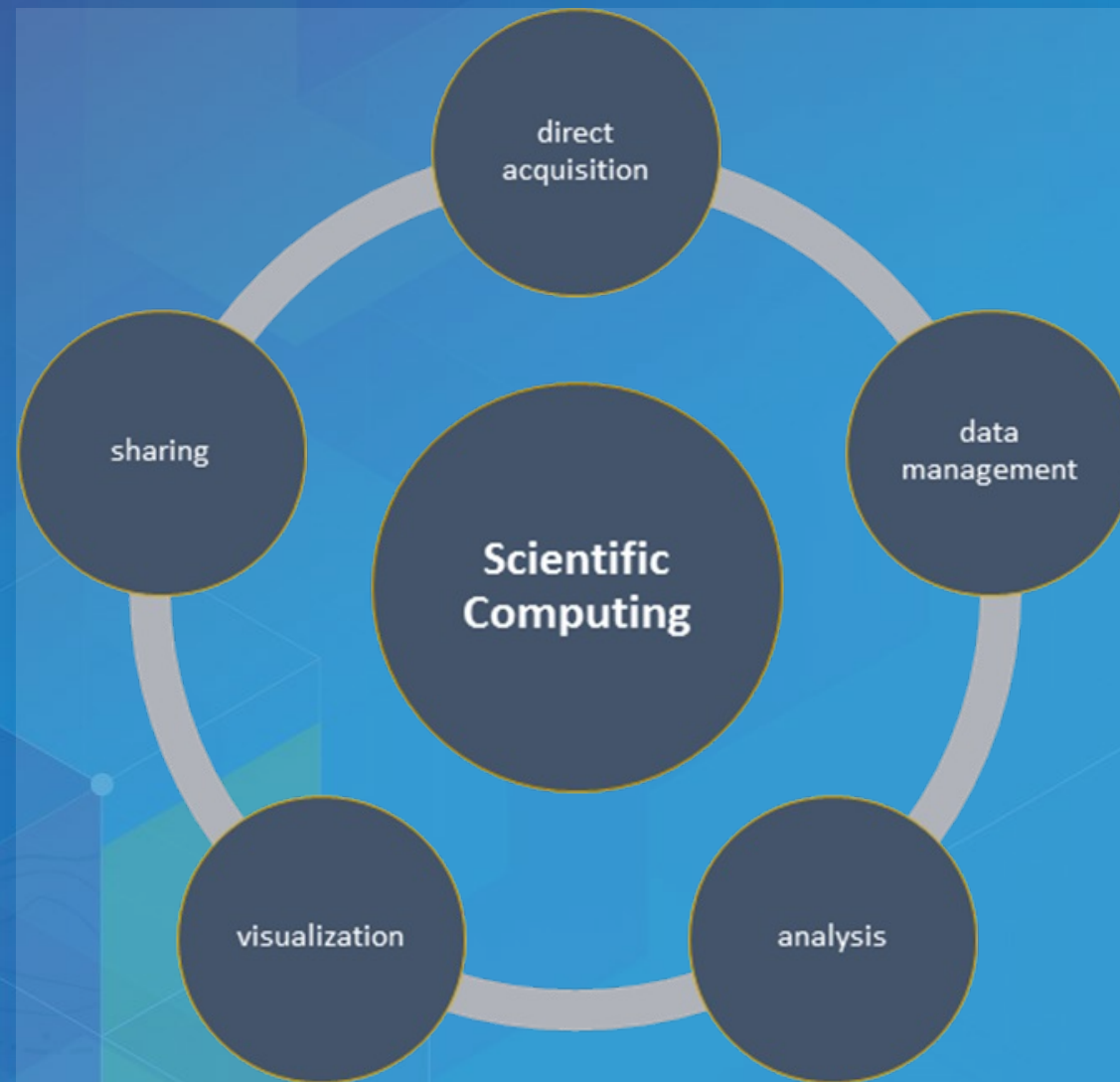
[Resources Section](#)



Scientific Computing



Scientific Computing



The application of computational methods to all aspects of the process of scientific investigation – data acquisition, data management, analysis, visualization, and sharing of methods and results.

Extending ArcGIS

- ArcGIS is a *system of record*. Combine data and analysis from many fields and into a common environment.
- Why extend? Can't do it all, we support over 1000 GP tools — enabling *integration* with other environments to extend the platform.

Python

Why Python?

- Accessible for new-comers, and the most taught first language in US universities
 - Extensive package collection (56k on PyPI), broad user-base
 - Strong glue language used to bind together many environments, both open source and commercial
 - Open source with liberal license — do what you want
-
- Brand new to Python? This talk may be challenging
 - Resources include materials that for getting started

Python in ArcGIS

- Python API for driving ArcGIS Desktop and Server
- A fully integrated module: `import arcpy`
- Interactive Window, Python Addins, Python Toolboxes
- Extensions:
 - Spatial Analyst: `arcpy.sa`
 - Map Document: `arcpy.mapping`
 - Network Analyst: `arcpy.na`
 - Geostatistics: `arcpy.ga`
 - Fast cursors: `arcpy.da`
- ArcGIS API for Python

Python in ArcGIS

- Python 3.5 in Pro ([Desktop vs Pro Python](#))
 - `arcpy.mp` instead of `arcpy.mapping`
- Continue to add modules: NetCDF4, xlrd, xlwt, PyPDF2, dateutil, pip
- [Python raster function](#), with a [repository of examples](#) using SciPy for on the fly visualizations

Python in ArcGIS

- Here, focus on SciPy stack, what's included out of the box
- Move toward maintainable, reusable code and beyond the “one-off”
- Recurring theme: multi-dimensional data structures
- Also see [Brendan Collins talk tomorrow](#) which covers `dask`

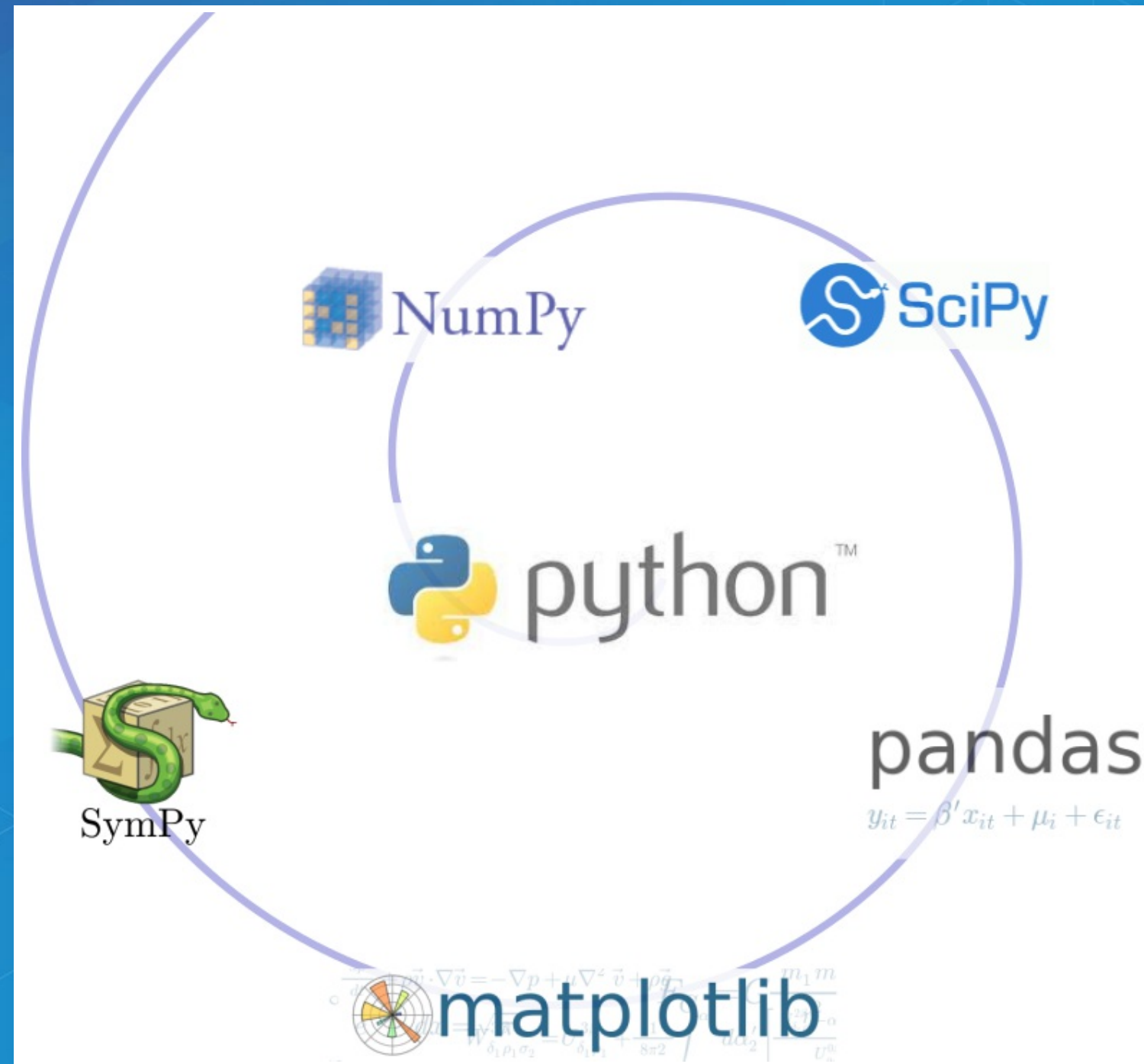
SciPy



Why SciPy?

- Most languages don't support things useful for science, e.g.:
 - Vector primitives
 - Complex numbers
 - Statistics
- Object oriented programming isn't always the right paradigm for analysis applications, but is the only way to go in many modern languages
- SciPy brings the pieces that matter for scientific problems to Python.

SciPy Stack



Included SciPy

Package	KLOC	Contributors	Stars
<u>matplotlib</u>	118	441	4909
<u>Nose</u>	7	75	1053
<u>NumPy</u>	236	429	4011
<u>Pandas</u>	183	408	8765
<u>SciPy</u>	387	387	2930
<u>SymPy</u>	243	443	3642
Totals	1174	1885	

Testing with Nose

- Nose — a Python framework for testing
- Tests improve your productivity, and create robust code
- Nose builds on `unittest` framework, extends it to make testing easy.
- Plugin architecture, includes a number of plugins and can be extended with third-party plugins.



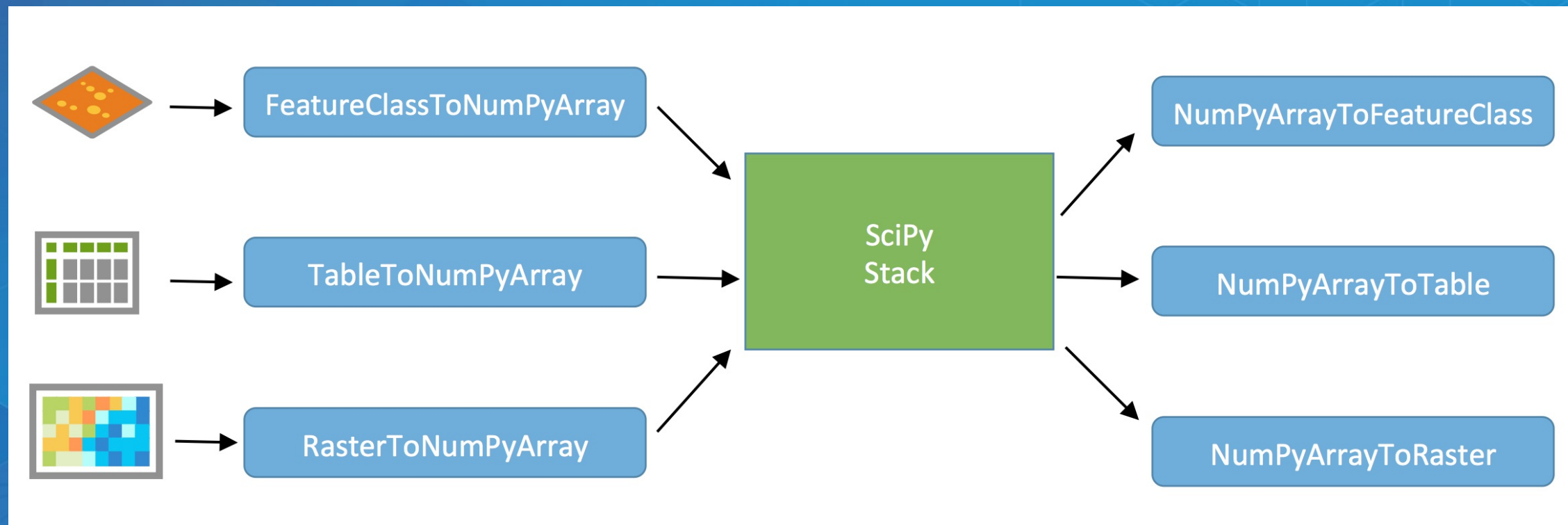
1. An array object of arbitrary homogeneous items
2. Fast mathematical operations over arrays
3. Random Number Generation

0	1	2	3	4	5
10	11	12	13	14	15
20	21	22	23	24	25
30	31	32	33	34	35
40	41	42	43	44	45
50	51	52	53	54	55

ArcGIS + NumPy

- ArcGIS and NumPy can interoperate on raster, table, and feature data.
- See [Working with NumPy in ArcGIS](#)
- In-memory data model. Example script to [process by blocks](#) if working with larger data.

ArcGIS + NumPy





Computational methods for:

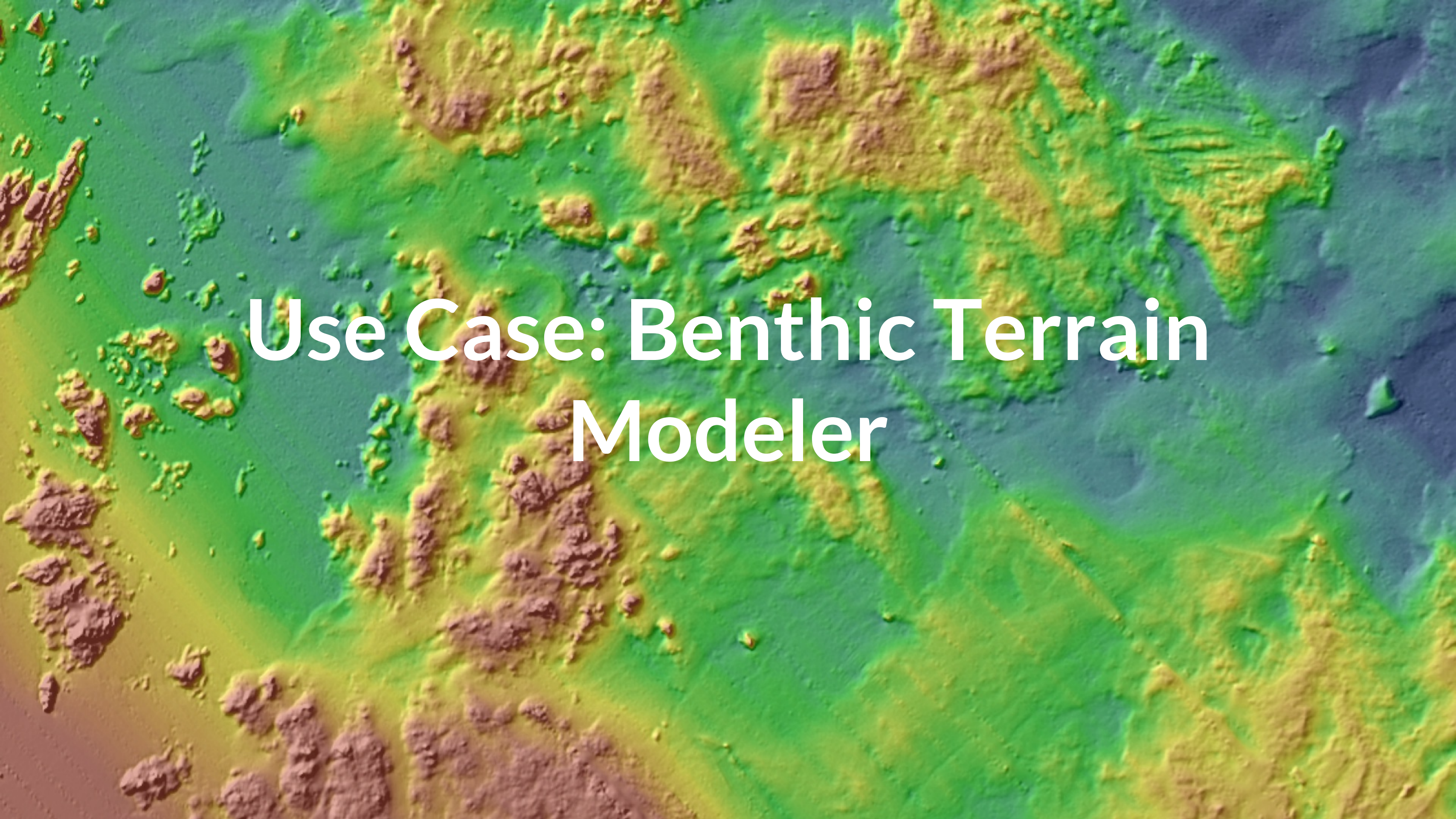
- Integration ([scipy.integrate](#))
- Optimization ([scipy.optimize](#))
- Interpolation ([scipy.interpolate](#))
- Fourier Transforms ([scipy.fftpack](#))
- Signal Processing ([scipy.signal](#))
- Linear Algebra ([scipy.linalg](#))
- Spatial ([scipy.spatial](#))
- **Statistics ([scipy.stats](#))**
- **Multidimensional image processing ([scipy.ndimage](#))**

SciPy: Geometric Mean

- Calculating a geometric mean of an *entire raster* using SciPy ([source](#))

$$\left(\prod_{i=1}^n a_i\right)^{1/n} = \sqrt[n]{a_1 \cdot a_2 \cdots a_n}$$

```
import scipy.stats
rast_in = 'data/input_raster.tif'
rast_as_numpy_array = arcpy.RasterToNumPyArray(rast_in)
raster_geometric_mean = scipy.stats.stats.gmean(
    rast_as_numpy_array, axis=None)
```

Use Case: Benthic Terrain Modeler

Benthic Terrain Modeler

- A Python Add-in and Python toolbox for geomorphology
- Open source, can borrow code for your own projects:
<https://github.com/EsriOceans/btm>
- Active community of users, primarily marine scientists, but also useful for other applications

Lightweight SciPy Integration

- Using `scipy.ndimage` to perform basic multiscale analysis
- Using `scipy.stats` to compute circular statistics

Lightweight SciPy Integration

[Example source](#)

```
import arcpy
import scipy.ndimage as nd
from matplotlib import pyplot as plt

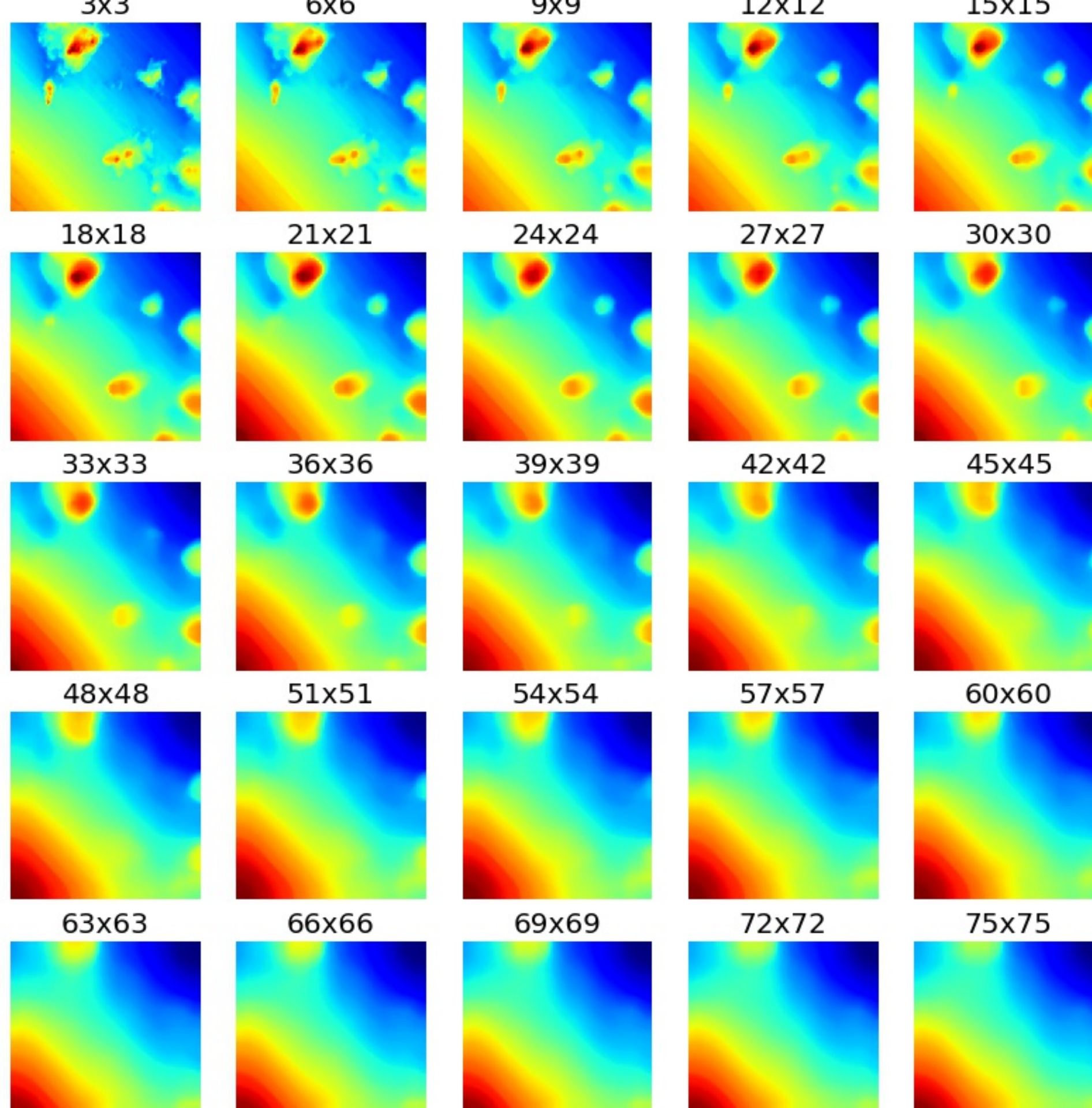
ras = "data/input_raster.tif"
r = arcpy.RasterToNumPyArray(ras, "", 200, 200, 0)

fig = plt.figure(figsize=(10, 10))
```

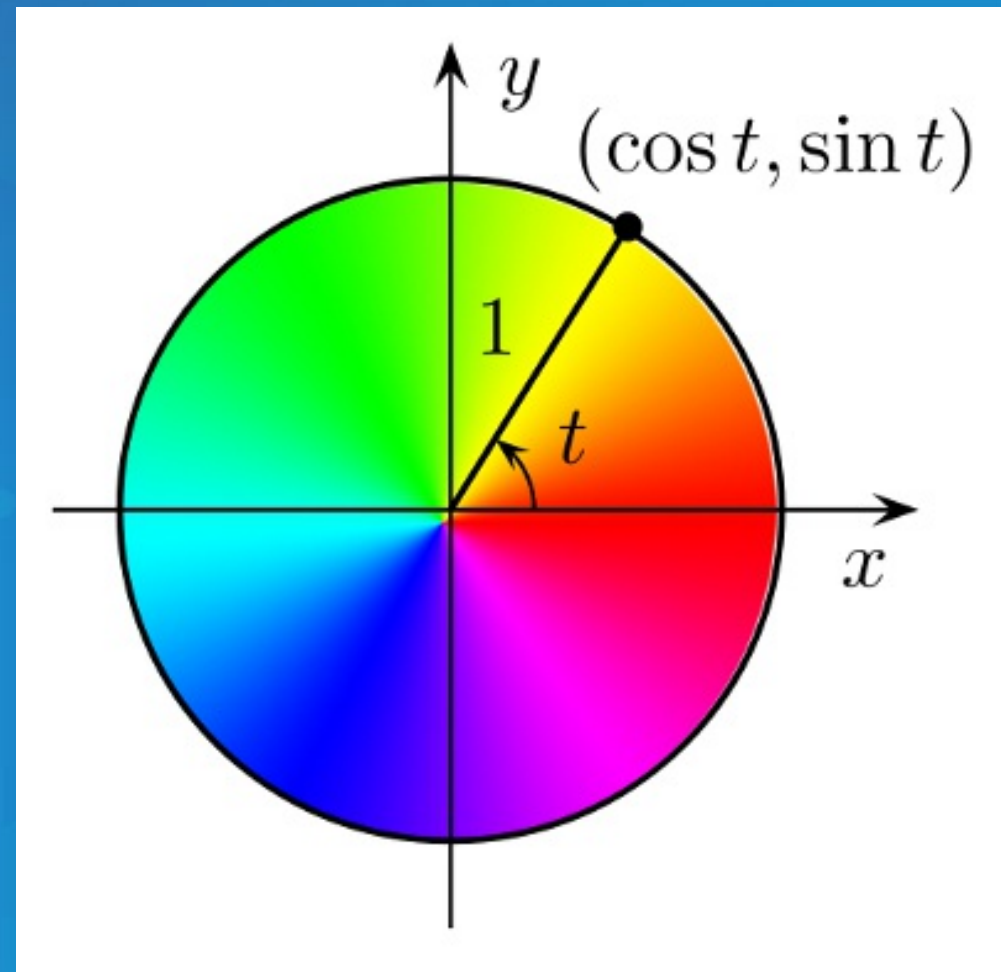
Lightweight SciPy Integration

```
for i in xrange(25):
    size = (i+1) * 3
    print "running {}".format(size)
    med = nd.median_filter(r, size)

    a = fig.add_subplot(5, 5,i+1)
    plt.imshow(med, interpolation='nearest')
    a.set_title('{}x{}'.format(size, size))
    plt.axis('off')
    plt.subplots_adjust(hspace = 0.1)
    prev = med
```



SciPy Statistics



- Break down aspect into `sin()` and `cos()` variables
- Aspect is a circular variable – without this 0 and 360 are opposites instead of being the same value

SciPy Statistics

Summary statistics from SciPy include circular statistics ([source](#)).

```
import scipy.stats.morestats

ras = "data/aspect_raster.tif"
r = arcpy.RasterToNumPyArray(ras)

morestats.circmean(r)
morestats.circstd(r)
morestats.circvar(r)
```

Demo: SciPy



Multidimensional Data

NetCDF4

- Fast, HDF5 and NetCDF4 read+write support, OPeNDAP
- Hierarchical data structures
- Widely used in meteorology, oceanography, climate communities
- Easier: Multidimensional Toolbox, but can be useful

[\(Source\)](#)

```
import netCDF4
nc = netCDF4.Dataset('test.nc', 'r', format='NETCDF4')
print nc.file_format
# outputs: NETCDF4
nc.close()
```


Multidimensional Improvements

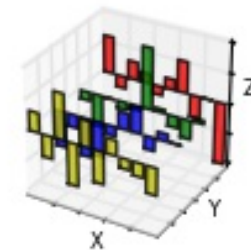
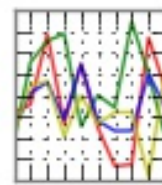
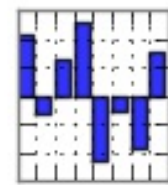
- Multidimensional formats: HDF, GRIB, NetCDF
- Access via OPeNDAP, vector renderer, Raster Function Chaining
- [An example which combines mutli-D with time](#)
- Multi-D supported as WMS, and in Mosaic datasets (10.2.1+)

Pandas



pandas

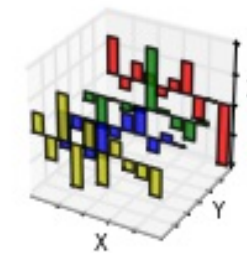
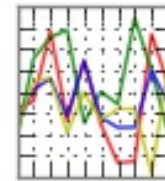
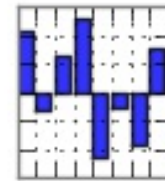
$$y_{it} = \beta' x_{it} + \mu_i + \epsilon_{it}$$



- Panel Data – like R "data frames"
- Bring a robust data *analysis* workflow to Python
- Data frames are fundamental – treat tabular (and multi-dimensional) data as a labeled, indexed series of observations.

pandas

$$y_{it} = \beta' x_{it} + \mu_i + \epsilon_{it}$$



([Source](#))

```
import pandas
```

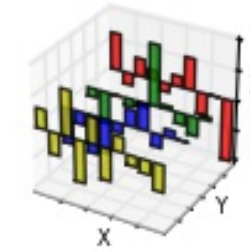
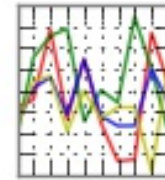
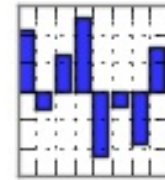
```
data = pandas.read_csv('data/season-ratings.csv')
```

```
data.columns
```

```
Index([u'season', u'households', u'rank', u'tv_households', \
       u'net_indep', u'primetime_pct'], dtype='object')
```


pandas

$$y_{it} = \beta' x_{it} + \mu_i + \epsilon_{it}$$



```
majority_simpsons = data[data.primetime_pct > 50]
```

	season	households	tv_households	net_indep	primetime_pct
0	1	13.4m[41]	92.1	51.6	80.751174
1	2	12.2m[n2]	92.1	50.4	78.504673
2	3	12.0m[n3]	92.1	48.4	76.582278
3	4	12.1m[48]	93.1	46.2	72.755906
4	5	10.5m[n4]	93.1	46.5	72.093023
5	6	9.0m[50]	95.4	46.1	71.032357
6	7	8.0m[51]	95.9	46.6	70.713202
7	8	8.6m[52]	97.0	44.2	67.584098
8	9	9.1m[53]	98.0	42.3	64.383562
9	10	7.9m[54]	99.4	39.9	60.916031
10	11	8.2m[55]	100.8	38.1	57.466063
11	12	14.7m[56]	102.2	36.8	53.958944
12	13	12.4m[57]	105.5	35.0	51.094891

Demo: Pandas



SymPy





- A Computer Algebra System (CAS), solve math equations ([source](#))

```
from sympy import *  
x = symbol('x')  
eq = Eq(x**3 + 2*x**2 + 4*x + 8, 0)
```

$$x^3 + 2x^2 + 4x + 8 = 0$$

```
solve(eq, x)
```

$$[-2, -2i, 2i]$$

Demo: SymPy



Where and How Fast?



Where Can I Run This?

- Now:
 - ArcGIS Pro (64-bit) Standalone Python Install for Pro
 - 10.4: ArcMap, Server, both 32- and 64- bit environments
 - Both now ship with Scipy Stack (sans IPython)
 - MKL enabled NumPy and SciPy everywhere
 - Older releases: NumPy: ArcGIS 9.2+, matplotlib: ArcGIS 10.1+, SciPy: 10.4+, Pandas: 10.4+
 - Conda for managing full Python environments, consuming and producing packages
 - With the ArcGIS API for Python! Can run anywhere Python runs.

How Does It perform?

- Built with Intel's [Math Kernel Library \(MKL\)](#) and compilers—highly optimized Fortran and C under the hood.
- Automated parallelization for executed code

[MKL Performance Chart](#)

from future import *

Opening Doors

- Machine learning (`scikit-learn`, `scikit-image`, ...)
- Deep learning (`theano`, ...)
- Bayesian statistics (`PyMC`)
 - Markov Chain Monte Carlo (MCMC)
- Frequentist statistics (`statsmodels`)
- With Conda, not just Python! `tensorflow`, many others

Resources

Other Sessions

- [Exploring Continuum Analytics' Open Source Offerings](#) – tomorrow 10:30 in Mesquite G-H
- [Getting Data Science with R and ArcGIS](#) – stick around, in this room in 30 min! [2016 video](#)
- [Integrating Open-source Statistical Packages with ArcGIS](#) earlier today, [2016 video](#)
- [Harnessing the Power of Python in ArcGIS Using the Conda Distribution](#) yesterday, [2016 video](#)

New to Python

- Courses:
 - [Programming for Everybody](#)
 - [Codecademy: Python Track](#)
- Books:
 - [Learn Python the Hard Way](#)
 - [How to Think Like a Computer Scientist](#)

GIS Focused

- [Python Scripting for ArcGIS](#)
- [ArcPy and ArcGIS - Geospatial Analysis with Python](#)
- [Python Developers GeoNet Community](#)
- [GIS Stackexchange](#)

Scientific

Courses:

- [Python Scientific Lecture Notes](#)
- [High Performance Scientific Computing](#)
- [Coding the Matrix: Linear Algebra through Computer Science Applications](#)
- [The Data Scientist's Toolbox](#)

Scientific

Books:

- Free:
 - [Probabilistic Programming & Bayesian Methods for Hackers](#)
 - very compelling book on Bayesian methods in Python, uses SciPy + PyMC.
 - [Kalman and Bayesian Filters in Python](#)

Scientific

- Paid:
 - [Coding the Matrix](#)
 - How to use linear algebra and Python to solve amazing problems.
 - [Python for Data Analysis: Data Wrangling with Pandas, NumPy, and IPython](#)
 - The canonical book on Pandas and analysis.

Packages

Only require SciPy Stack:

- Scikit-learn:
 - [Lecture material](#)
 - Includes SVMs, can use those for image processing among other things...
- FilterPy, Kalman filtering and optimal estimation:
 - [FilterPy on GitHub](#)
- [An extensive list of machine learning packages](#)

Code

- [ArcPy + SciPy on Github](#)
- [raster-functions](#)
 - An open source collection of function chains to show how to do complex things using NumPy + scipy on the fly for visualization purposes
- [statistics library](#) with a handful of descriptive statistics included in Python 3.4.
- *TIP:* Want a codebase that runs in Python 2 and 3? [Check out future](#), which helps maintain a single codebase that supports both. Includes the `futurize` script to initially a project written for one version.

Scientific ArcGIS Extensions

- [PySAL ArcGIS Toolbox](#)
- [Movement Ecology Tools for ArcGIS \(ArcMET\)](#)
- [Marine Geospatial Ecology Tools \(MGET\)](#)
 - Combines Python, R, and MATLAB to solve a wide variety of problems
- [SDMToolbox](#)
 - species distribution & maximum entropy models
- [Benthic Terrain Modeler](#)
- [Geospatial Modeling Environment](#)
- [CircuitScape](#)

Conferences

- [PyCon](#)
 - The largest gathering of Pythonistas in the world
- [SciPy](#)
 - A meeting of Scientific Python users from all walks
- [GeoPython](#)
 - The Python event for Python and Geo enthusiasts
- [PyVideo](#)
 - Talks from Python conferences around the world available freely online.
 - [PyVideo GIS talks](#)

Closing



Thanks

- Geoprocessing Team
- The many amazing contributors to the projects demonstrated here.
 - Get involved! All are on GitHub and happily accept contributions.

Rate This Session

iOS, Android: Feedback from within the app

Windows Phone, or no smartphone? Cuneiform tablets accepted.





esri

THE
SCIENCE
OF
WHERE