Scientific Programming with the SciPy Stack

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https://github.com/scw/scipy-devsummit-2016-talk

Handout PDF

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.

A minute or so for Kevin to talk about this.

Python

Why Python?

- Accessible for new-comers, and the most taught first language in US universites
- 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

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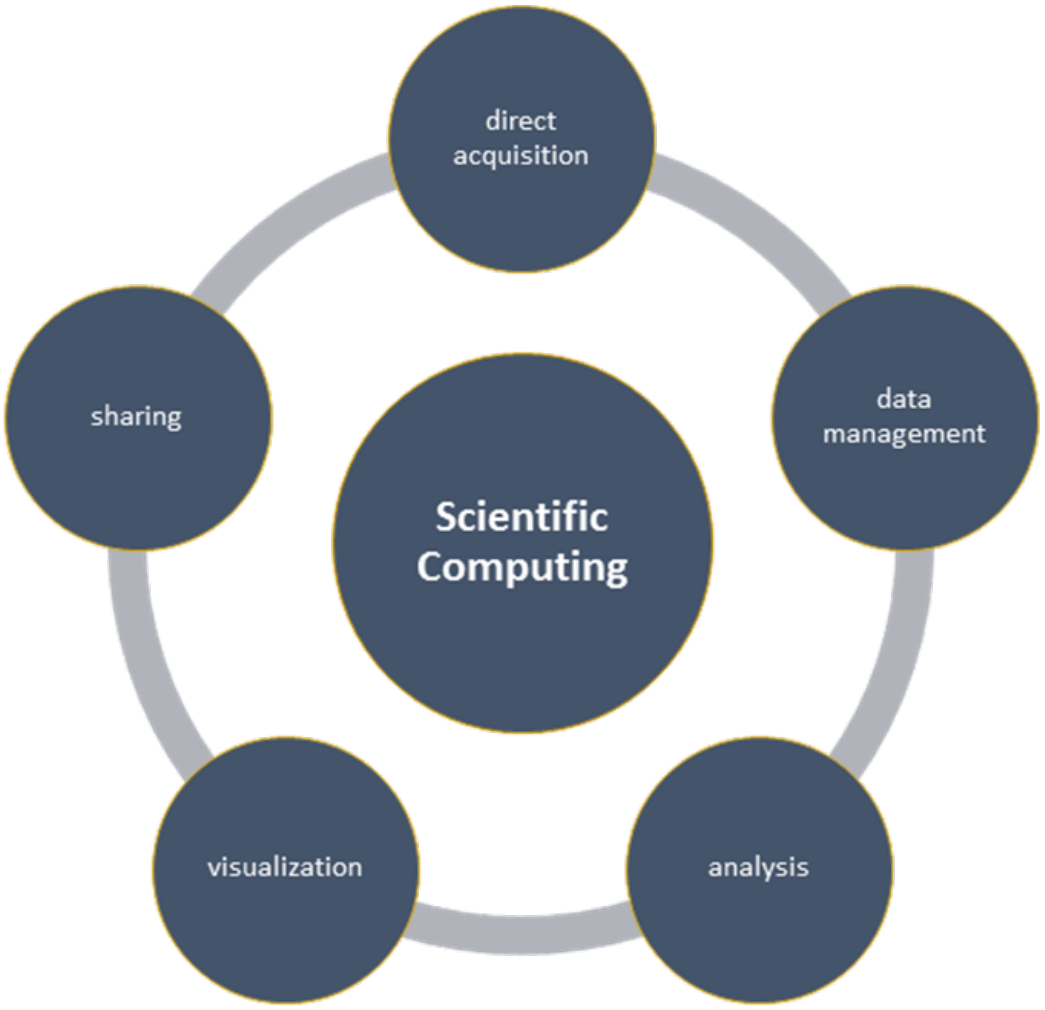

direct acquisition
data management
analysis
visualization
sharing
Scientific Computing

Figure 1:

- 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 Tooboxes
- Extensions:
  - Spatial Analyst: `arcpy.sa`
  - Map Document: `arcpy.mapping`
  - Network Analyst: `arcpy.na`
  - Geostatistics: `arcpy.ga`
  - Fast cursors: `arcpy.da`

Python in ArcGIS

- Python 3.4 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
- `arcpy.mp` Pro works with a conceptual model with *Project* at the root, so this module reflects that difference from ArcMap where *map document* is the root with `arcpy.mapping`.
- Modules galore: NetCDF4, xlrd, xlwt, PyPDF2, dateutil, pip, …

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
- Related talks today:
  - Getting Data Science with R and ArcGIS
    - 2:30PM, this room (Santa Rosa)

  - Python in ArcGIS Using the Conda Distribution
    * 4:00PM, Mesquite GH

Multi-dimensional data structures – numpy, pandas, our multi-d support all take advantage of different forms of an N-dimensional data structure. Rich, lets you pack simpler data into it for performance, still useful for 1D and 2D data!

PLUG ALERT: both talks I'm part of

Both also available online after the conference videos are posted to video.esri.com.

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.

Included SciPy

Package	KLOC	Contributors	Stars
matplotlib	118	426	3359
Nose	7	79	912
NumPy	236	405	2683
Pandas	183	407	5834
SciPy	387	375	2150
SymPy	243	427	2672
Totals	1174	1784	

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

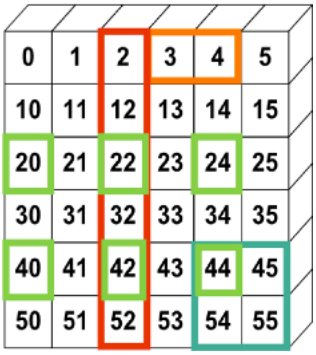


Figure 2:

SciPy Lectures, CC-BY

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

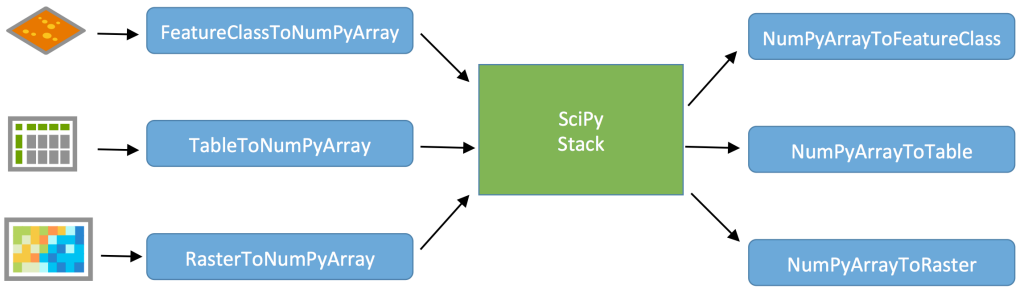


Figure 3:

matplotlib

- Plotting library and API for NumPy data
- Matplotlib Gallery

SciPy

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)

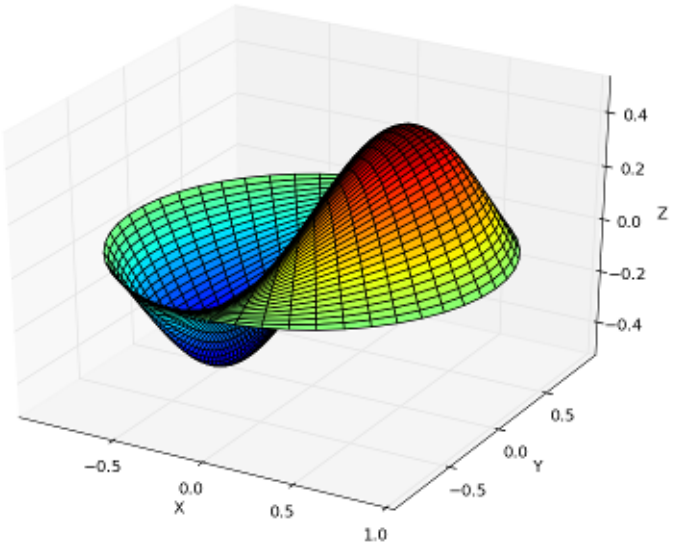


Figure 4:

- **Statistics** (scipy.stats)
- **Multidimensional image processing** (scipy.ndimage)

Spatial is the tools across all of the domains of science, very general.

That said, can be useful in a variety of circumstances, e.g. `KDTree` for finding data quickly.

SciPy: Geometric Mean

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

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

Figure 5:

```
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)
```

(Inspiration)

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

plt.savefig("btm-scale-compare.png", bbox_inches='tight')
```

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)
```

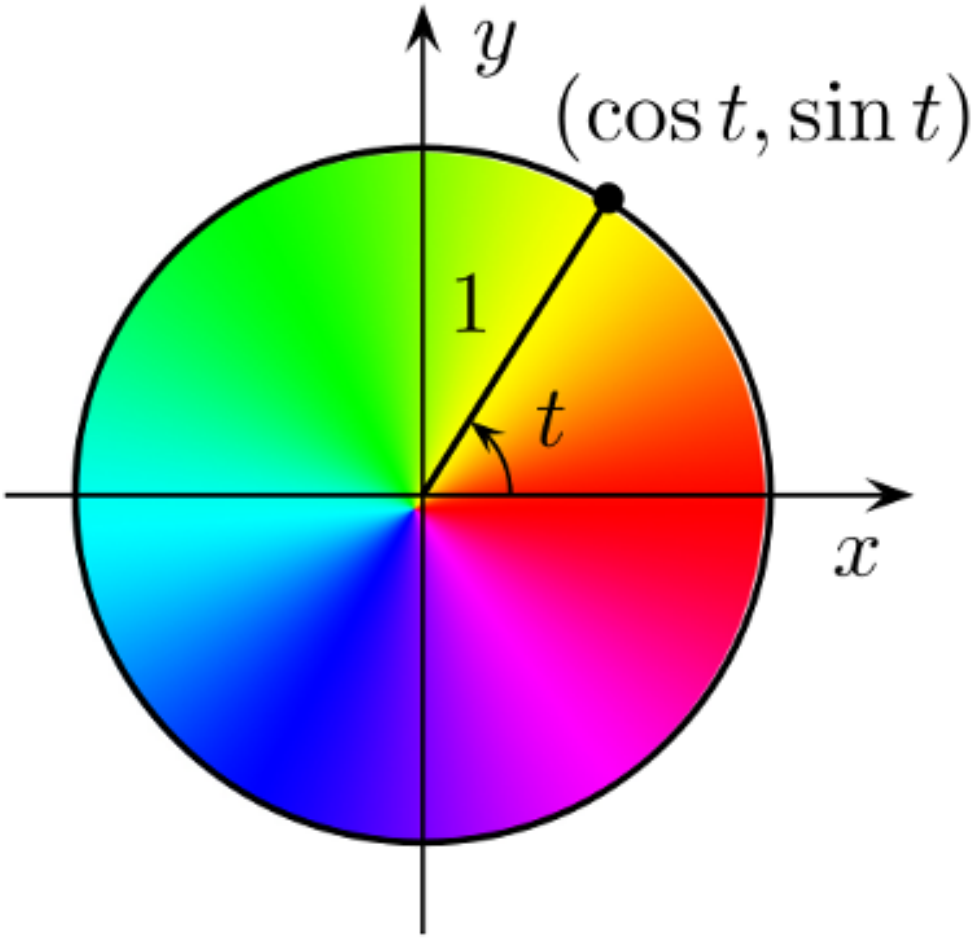


Figure 6:

Demo: SciPy

Multidimensional Data

NetCDF4

- Fast, HDF5 and NetCDF4 read+write support, OPeNDAP
- Heirarchical data structures
- Widely used in meterology, 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()
```

- CF compliant data
- Fast, C-based access

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

- **Pan**el **Da**ta — 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.

(Source)

```
import pandas

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

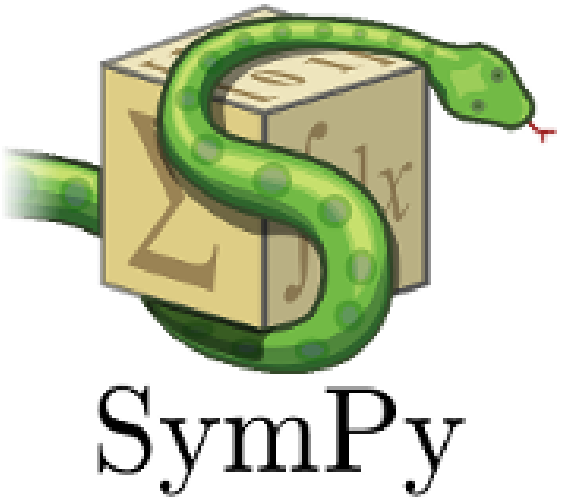
```
Index([u'season', u'households', u'rank', u'tv_households', \
       u'net_indep', u'primetime_pct'], dtype='object')
```


```
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

Pandas Demo

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)
```

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

Figure 7:

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

$$\left[-2, \quad -2i, \quad 2i\right]$$

Figure 8:

SymPy Demo

Where and How Fast?

Where Can I Run This?

- Now:
  - ArcGIS Pro (64-bit) Standalone Python Install for Pro
  - ArcGIS Desktop at 10.4: 32-bit, Background Geoprocessing (64-bit), Server (64-bit), Engine (32-bit)
    * 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+
- Upcoming:
  - IPython
  - Conda for managing full Python environments

```
- SciPy stack is now available across the platform. Try it out, you can build things th
- IPython: Let's get this done like yesterday. Had it in the 'upcoming' of last years s
- Conda session today, Mesquite GH at 4pm.
```

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

Quoting Kevin from last year: Wicked fast. Pandas is fast, scipy functions are fast, and we now enable MKL across the platform for all builds. You write Python, but get best of class performance for free.

Take this graph with a large grain of salt. Realistically, can expect 2-10x improvements in many numerical routines.

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`)

Resources

Other Sessions

- Harnessing the Power of Python in ArcGIS Using the Conda Distribution
- Getting Data Science with R and ArcGIS
- Automated Land Surface Temperature Estimation Using Python and ArcGIS Pro
- Writing Image Processing Algorithms using the Python Raster Function
- Python: Working with Scientific Data
- Python: Developing Geoprocessing Tools
- Integrating Open-source Statistical Packages with ArcGIS

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 cannonical 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

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Windows Phone, or no smartphone? Cuneiform tablets accepted.

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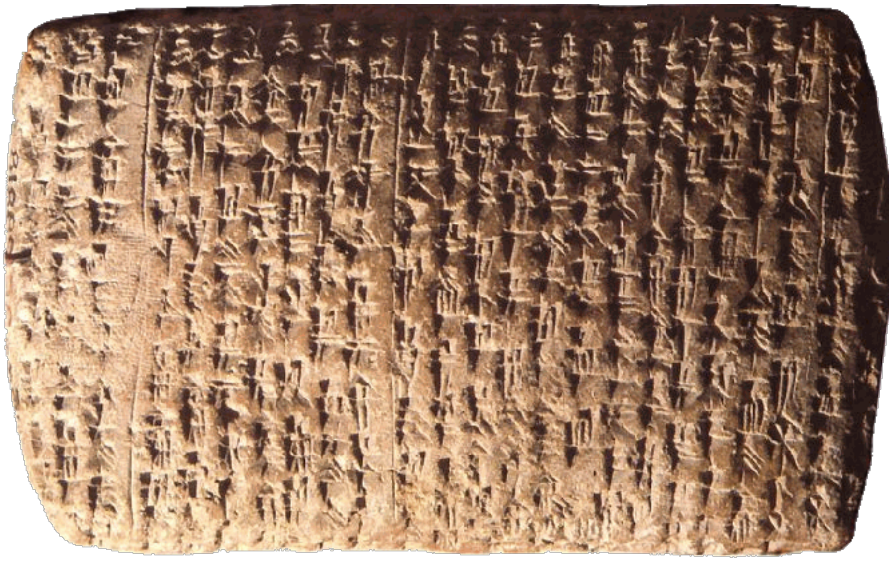

Figure 9: