What is Scipy?

Tool suite: Numpy, Scipy, matplotlib, IPython

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What is Scipy?

- a project, a library, a team, a community
- a tool suite for Python, written in C
- **Numpy**: arrays (stable, linear algebra, basic algorithms)
- **Scipy**: scientific library (large suite of tool boxes)
- **matplotlib**: powerful plotting with MATLAB-like syntax
- **IPython**: interactive, tab completion, distributed, readline, `matplotlib` integration

Scipy Packages

- `cluster`: Clustering, Vector Quantization
- `fftpack`: Fast Fourier Transforms (FFT Pack)
- `linalg`: Linear Algebra (BLAS, LAPACK, ATLAS)
- `sparse`: Sparse Matrices and Linear Algebra (UMFPack)
- `stats`: Random Numbers, Distribution Manipulations, Density Estimation, Moment Calculation

Scipy Packages

- `integrate`: numerical integration (quadrature)
- `optimize`: optimization (LP, QP, QCP)
- `signal`: signal processing, basic filters, wavelets
- `ndimage`: image processing, edge detection, morphology, image statistics, connected components, convolution, etc.
- `weave`: C/C++ integration with multiline strings for prototype code you can't vectorize

Scikits

- non-BSD licenses allowed (GPL, LGPL, etc.)
- still deciding on structure, packaging, standards; web page needs work
- `ann`: interface to the popular approximate nearest neighbor library. Very fast.
- `audiolab`: processing audio waveforms. Lots of formats.
- `learn`: machine learning
- `delauney`: Voronoi tesselations and Delauney triangulations

Scientific Computing in C

- GNU Scientific Library (GSL): free software, very stable, lots of features
- Numerical Recipes: restrictive licensing
- great for production systems
- hard to collaborate: some mathy friends are C-phobic
- syntax isn’t so succinct
- efficient

Scientific Computing in C

- high-level manipulative code is difficult but low-level is stuff is efficient and intuitive!
- Clean Python and C integration: the best of both worlds, just
  - write low-level vectorizable algorithms in Python
  - write low-level non-vectorizable algorithms in C
  - write high-level manipulative code in Python

Free Scripting Languages for Scienc

- **Octave and Scilab** (MATLAB-like)
- **R**: primarily for statistics. Very functional-oriented. Not efficient for large data.
- hard to write extensions
- confined to small programs
- *good* for *prototyping* algorithms
- *difficult* for developing larger *systems*
- based on old languages (MATLAB, 1982) and (S, S+, 1975, 1988)

Why I don't like MATLAB?

- proprietary: hard to collaborate–collaborators need licenses
- licenses: per-machine, not per-user. As project grows, more licenses needed - $$$.
- one needs lots of toolboxes, one for each machine - more $$$.
- pass-by-value: makes large data sets painful; slows programs
- *global variables*: hack introduced to get around pass-by-value. Makes code hard to maintain.

Why I don't like MATLAB?

- encourages interactive workflow. Batch scripting is difficult: reproducability of experiments and plots?
- hard to code rich data structures: trees, graphs, heaps, lists
- MATLAB forum code: lots of code. Not well organized. Some good code. Lots of sloppy code.
- not condusive to developing open source packages. Subcommunities are rare.

Why I don't like MATLAB?

- hard to organize MATLAB code into one coherent package. Must traverse lots of files for small modules. Code not organized into modules.
- we need OO to organize large scale systems
- *we do object-oriented*: yeah, sure you do.
  - must create a directory for every class
  - a file for every function.
  - objects are immutable. Changing involves a copy.
- one function/file: hard to organize code

Why I don’t like MATLAB?

- large scale cluster computing is limited: licenses, bloated minimal memory footprint, starting is slow, crashes require restarts taking time
- packages for coordinating large jobs: must buy another toolbox
- no cvs update: bug fixes, new tools are not immediate
- black box: can’t track down why MATLAB crashes.

Why I don’t like MATLAB?

- can’t contribute code back–no larger open source community. MATLAB is evolved on Mathworks’ terms, not the user/scientist.
- MATLAB is very numeric-specific. Python is more universal.
- GUI and database toolkits don’t come with it
- parsing files is difficult based on old fscanf technology
- hard to work with non-matrix data sets (e.g. web data, text)

Why I don't like MATLAB?

- mex is clunky: a lot of infrastructure is needed for a single external function. Documentation is incomplete.
- hard to wrap existing C libraries (e.g. GDAL). Must write large collection of wrappers.
- hard to debug mex C code
- hard to install on new machines. Sysadmins are sometimes needed to communicate with MATLAB sales office.

Why not Octave/Scilab?

- They aren't universal languages
- Hard to write large applications–languages not designed for it (e.g. pass-by-value, global variable hacks)
- Thin spread: must focus on *both* language and interpreter design and science code
- Python/Scipy: separation of concerns
  - **python team**: focus on developing the language and base tools.
  - **Scipy team**: focus on developing large science toolset.

Why not Octave/Scilab?

- Not as much as external code is available as with python.
- Wrapping C libraries is difficult. MEX interface not intuitive.
- Richer data structures (e.g. trees) not available.

Why Scipy?

- free: easy-to-collaborate
- open source: you're part of community, no black box
- python
  - universal: lots of people know and trust it
  - flexible: easy to do simple tasks
  - object-oriented: designed for writing applications
  - large corpora of packages: cross cuts many fields and problem domains

Why Scipy?

- fast: C implementation of core code
- succinct syntax: python's operator overloading `[]`, `*`, `-`, `**`, and yes lots of in-place operators `**=`.
- crazily flexible indexing–key to Numpy's success.
- lots of ways to vectorize (more than MATLAB?)
- in-place algorithms are easy with pass-by-reference and in-place operators

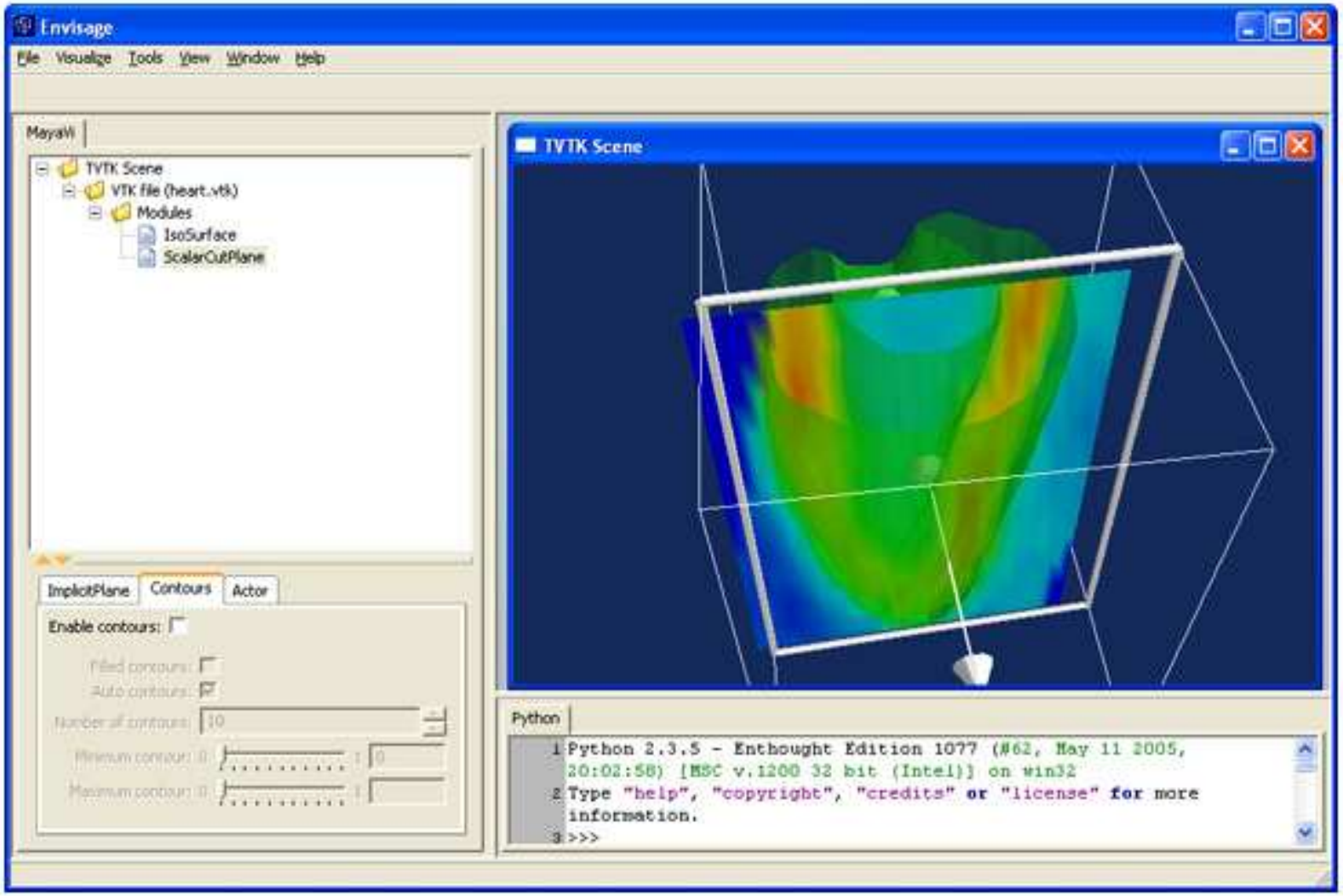
Why Scipy?

- rich data structures: text, graphs, trees, hash maps
- powerful parsing: binary file unpacking, text parsing
- network I/O
- GUI building
- dot notation is intuitive (e.g. `(X < 0).mean()`, arrays are objects

Learning Curve

- easy to transition from MATLAB, minor differences. Arrays are
  - Python objects, implemented in C for efficiency
  - not copied when sliced, reshaped or transposed
  - sliced with square brackets (instead of parentheses)
  - indexable with lists of indices and boolean arrays
  - reshapable to flat views with `.ravel()`

Large Applications



Large Applications

- large data repository? no problem: MySQL databases
  - store terabytes of astronomy data. Queries returned as numpy arrays.
  - geospatial images organized by georeference queries
- GUI Building: Qt, GTK, Tcl – take your pick!
- C and C++ extensions are easy!
- Existing C libraries getting wrapped all the time!

Why Scipy?

- Quick migration from MATLAB
  - differences are largely semantic: values are references to arrays
  - personal experience: 15,000+ lines converted to Python/Scipy in three months
  - lots of functions w/ same calling convention
- Seamless interactive and batch processing
- Easy to *prototype* – no need to rewrite prototypes

Why Scipy?

- Weave and Cython: write C/C++ in Python!
- multi-threading with pyprocessing
- parallelized interactivity with new IPython1
- wrapping existing C libraries is easy:

```
# in python
from ctypes import load_library
mylib = load_library("/usr/lib/mylib.so")
mylib.compute(myArray.ctypes.data)
```

Scipy Community

- Vibrant, friendly, and helpful.
- Scipy serves science.
- Scientists represent the bulk of the community.
- Enthought is available for hire: let your science money shape Scipy's future.

Scipy Community

- lots of software packages depend on Scipy base tools: distributed computing, bioinformatics, geospatial, brain imaging, aeronautics, financial, physics, commercial end-user applicances, etc.

Onward!

Onward to demo! Let's see Scipy in action by playing with it at an IPython prompt. We will use matplotlib for plotting.