The Development and Future of Python at STScI

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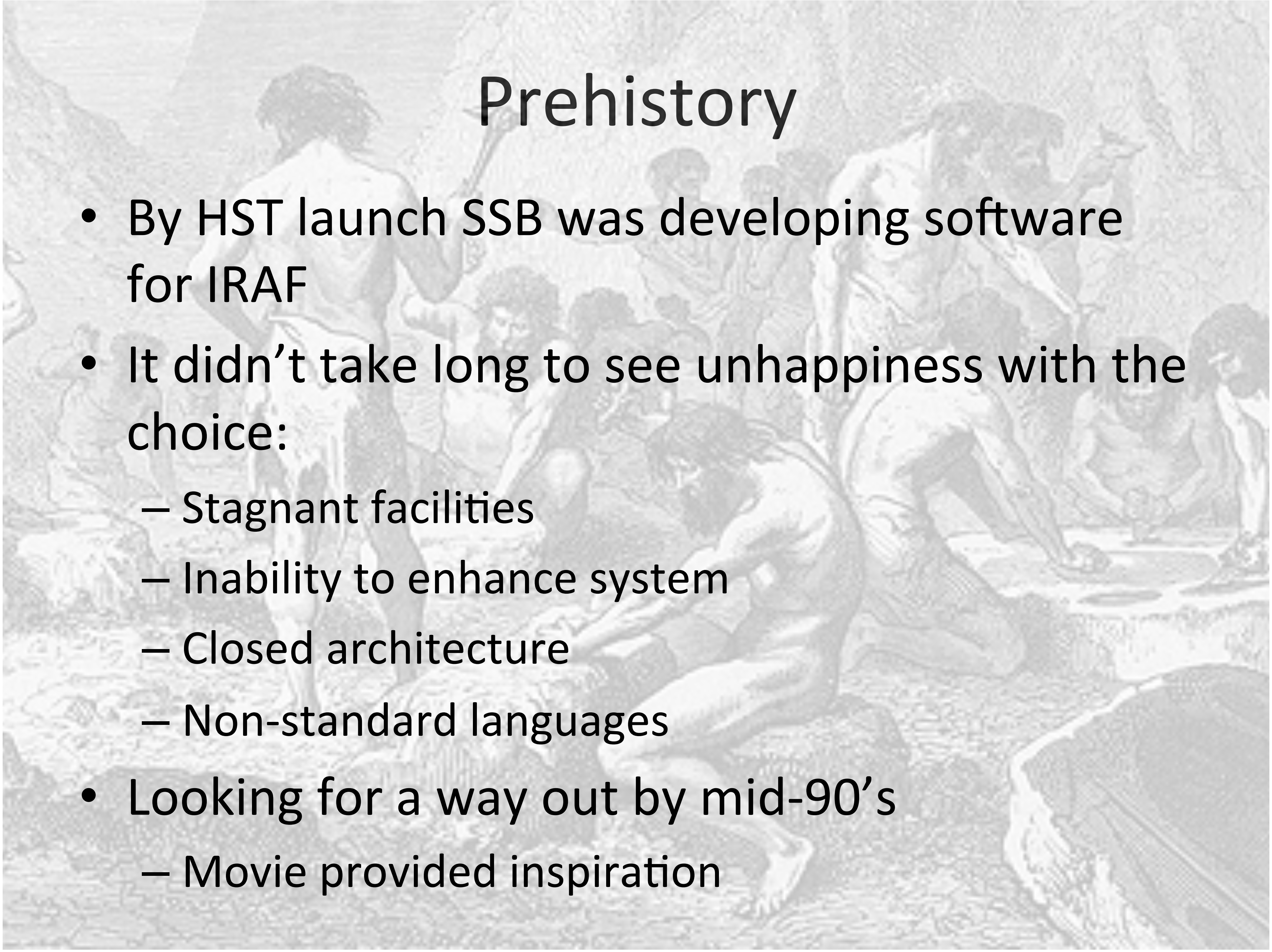
Outline

- Pre-Python History
- Python History
- Role for JWST
- Current work
- Challenges



Prehistory

- By HST launch SSB was developing software for IRAF
- It didn’t take long to see unhappiness with the choice:
  - Stagnant facilities
  - Inability to enhance system
  - Closed architecture
  - Non-standard languages
- Looking for a way out by mid-90’s
  - Movie provided inspiration

Foot in the door

- PyRAF: Sold as a better IRAF CL
- Python at the time was the only reasonable choice for a scripting language
- The big surprise was that it was a fantastic development language too. We wanted to write everything in it.
- But that meant lots of basic tools were needed to allow that

But Really, Why Python?

- Gives us an excuse to watch Monty Python and purchase related paraphernalia
- It's fun to use
- Excuses use of silly names
- Escape from IRAF

Slightly more seriously

- Escape from IRAF
- Out-IDL IDL
- Unify developer and astronomer languages
- Leverage much broader efforts available
- More satisfaction developing
  - increase “moxie factor”
- Avoids Møøse bites

Basic Foundations Needed

- Better array tools
  - Numeric at that time, but not good enough
  - → numarray → numpy
- Efficient and powerful way of reading and writing FITS files.
  - No complete tool available
  - Adapted and expanded Paul Barrett's pyfits
- Visualization
  - the situation was a mess
  - → chaco → matplotlib

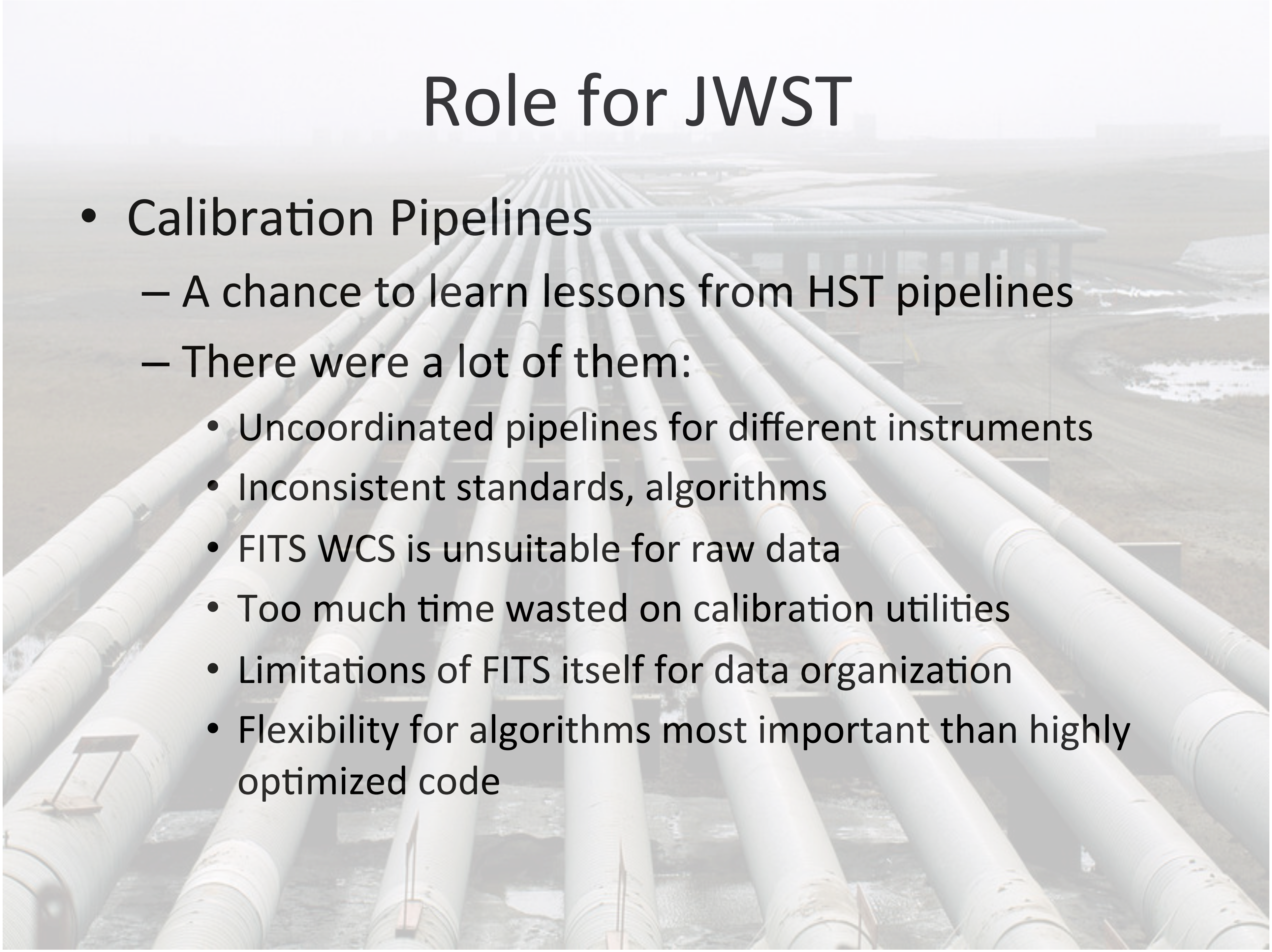
Initial use of Python

- HST pipelines and associated software
  - CALCOS
  - Multidrizzle/astrodrizzle
  - Pysynphot
- Rewrote Java-based ETCs in Python
  - Though not just for the hell of it

Data Analysis demands more

- Operations uses are comparatively narrow
- General data analysis requires much broader toolset that is easier for astronomers to use.
- Large numbers of existing tools for IRAF without corresponding tools in Python.
- Tools need to be broader than just what HST and JWST need.
- HST never really had resources to fund this
- JWST now comes into the picture.

Role for JWST



- Calibration Pipelines
  - A chance to learn lessons from HST pipelines
  - There were a lot of them:
    - Uncoordinated pipelines for different instruments
    - Inconsistent standards, algorithms
    - FITS WCS is unsuitable for raw data
    - Too much time wasted on calibration utilities
    - Limitations of FITS itself for data organization
    - Flexibility for algorithms most important than highly optimized code

Role for JWST (continued)

- Data Analysis:
  - – Needed tools to support new modes HST didn’t have:
    - MOS and IFU spectroscopy
  - – Launch delay provided an opportunity for more systematic attempt to provide a more complete suite of data analysis tools
    - Did we really want to depend on IRAF to the end of the mission?
    - i.e., we need to replace most useful IRAF capabilities

The Good

- Request to fund “IRAF replacement” well funded.
- Significant resources added (~ 5 people over 5 years or so)
- Very unusual to see this kind of support for Data Analysis work.

But…

The Bad

- Such resources are vulnerable to:
  - Priority demands
  - Political needs
  - Budget problems
  - Decreasing HST support
- Potentially worse:
  - Process entanglement

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Digression: what works and what doesn’t

- Successful (IMHO):
  - IRAF/STSDAS/TABLES
  - IDL/astrolib
  - AIPS
  - Sherpa
  - MIDAS
  - PyRAF, pyfits, numarray/numpy, matplotlib, astropy
  - None of these had a heavy formal “Program Management” development process (at least to start). Some had virtually none at all.

Digression continued

- Unsuccessful (circumspection requires that I be somewhat vague.)
  - Early HST DA efforts (pre-launch); all tossed out.
  - [redacted] ++
  - [redacted] Data Analysis project
  - Most US [redacted] -related DA projects
- All these had heavy Program Management processes
  - No doubt there are other factors, and
  - It may just be a coincidence, but nevertheless…

Astropy born in 2011

JWST Data Analysis plans

General issues:

- Significant overlap with Calibration Pipeline needs
- Make it generic as possible
  - – If not able to fill in all needs, make it as easy as possible for others to do so.
    - E.g., supply templates and examples of how to do so
- Use Astropy as the focus (either in core or as affiliated packages)

JWST Plans: Core capabilities

- More useful WCS library
  - FITS standard is a very inflexible model
  - Essentially unusable for distorted data
  - Aids increasing desire to avoid resampling
- A more useful data format than FITS (ASDF)
  - We need this to store the new WCS info anyway
  - Easy to generalize to cover most FITS use cases.
- Modeling/Fitting
  - Useful in many contexts for JWST

JWST Plans: Core tools

Supporting (among other things):

- Spectral cube visualization and analysis
- Multi-Object Spectroscopy visualization and analysis
- Spectral model fitting
- PSF matching and related PSF tools
- Coronagraph reduction tools
- Image Utilities
- Source identification and characterization tools

Philosophy

- Replace important IRAF functionality, but not necessarily the same approach.
- Rather than large black-box tasks, a layered approach of useful low, medium, and high-level libraries and tasks.
- Leverage existing functionality in scipy and other existing packages
  - But may need to wrap to present a consistent and convenient interface for astronomers.

Dealing with Interactive Use

- Important use case, but
- GUIs are very, very expensive to develop
  - Complex ones can be 10X more work than command line equivalent functionality
  - Very easy to waste a lot of resources with mistakes in design choices
  - Early and fast progress gives a false impression of the total amount of work required
    - Effort grows very nonlinearly
  - Basic design and technical decisions here have long-standing consequences.
  - One of my biggest worries.
  - Need to be very tough about allowing feature growth
    - Rely on plug-ins for extending functionality
- While comparatively primitive, IRAF dealt with this issue in a very smart and economical way.
  - Possibly the fallback approach.

Basic GUI questions

- What underlying technology to use?
- Web-based vs desktop GUI?
- Web pros:
  - Avoids installation issues regarding GUI framework
  - Much of GUI development moving that way
  - Makes remote use very easy (e.g., server side computations)
- Web cons:
  - Implies lots of development in Javascript
  - Can one really wall off what needs to be in JS?
    - Is there a slippery slope of re-implementing many tools already in Python?
  - Raises potential performance issues.

Basic GUI questions (cont.)

- Desktop GUI pros:
  - No need to use Javascript
  - Avoids potential Python/Javascript interface and performance issues
  - Existing tools mostly available as desktop GUIs
- Desktop GUI cons:
  - Frameworks can be difficult installs
  - Dwindling interest in general?
- Decision: Desktop GUI for now
  - Easiest way to show lots of initial progress
  - Binary packagers solve most of the installation issues (e.g., Anaconda)
  - Users need to install Python anyway, so in this case web interface doesn’t avoid users having to install software.

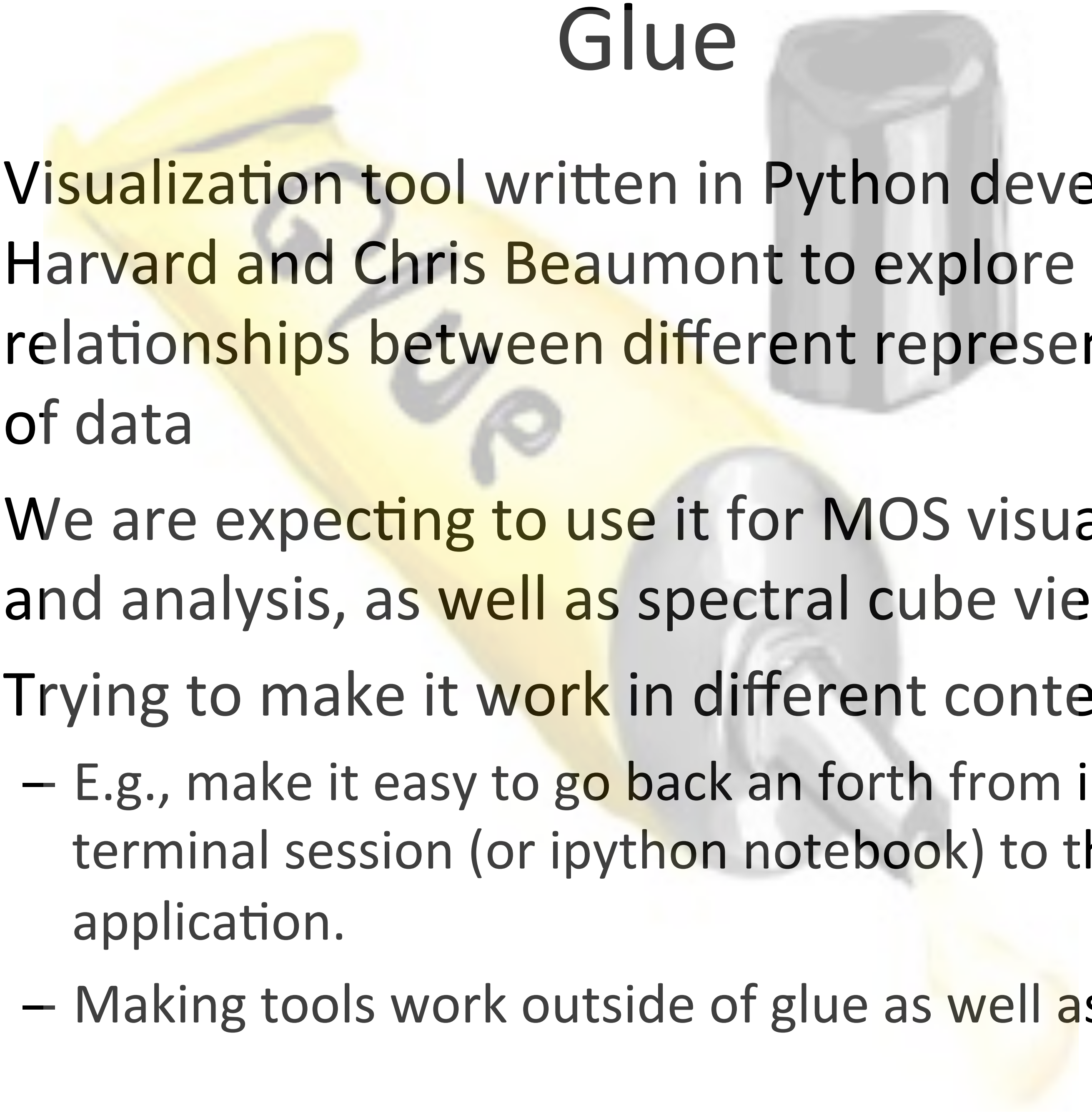
Desktop GUI issues

- Qt is the obvious choice (for now)
- Modern interface with many features and tools
- Cross platform (supports all common OS's)
- Used by the tools we are most interested in adopting, namely:
  - Glue
  - Ginga
- Reusing these should save a lot of effort. Both are written in Python

Ginga

- Basic, responsive Image viewer developed by Erik Jescke at Suburu.
- Well set up to handle plug-ins for customized applications
- Can be used within Glue!

Glue

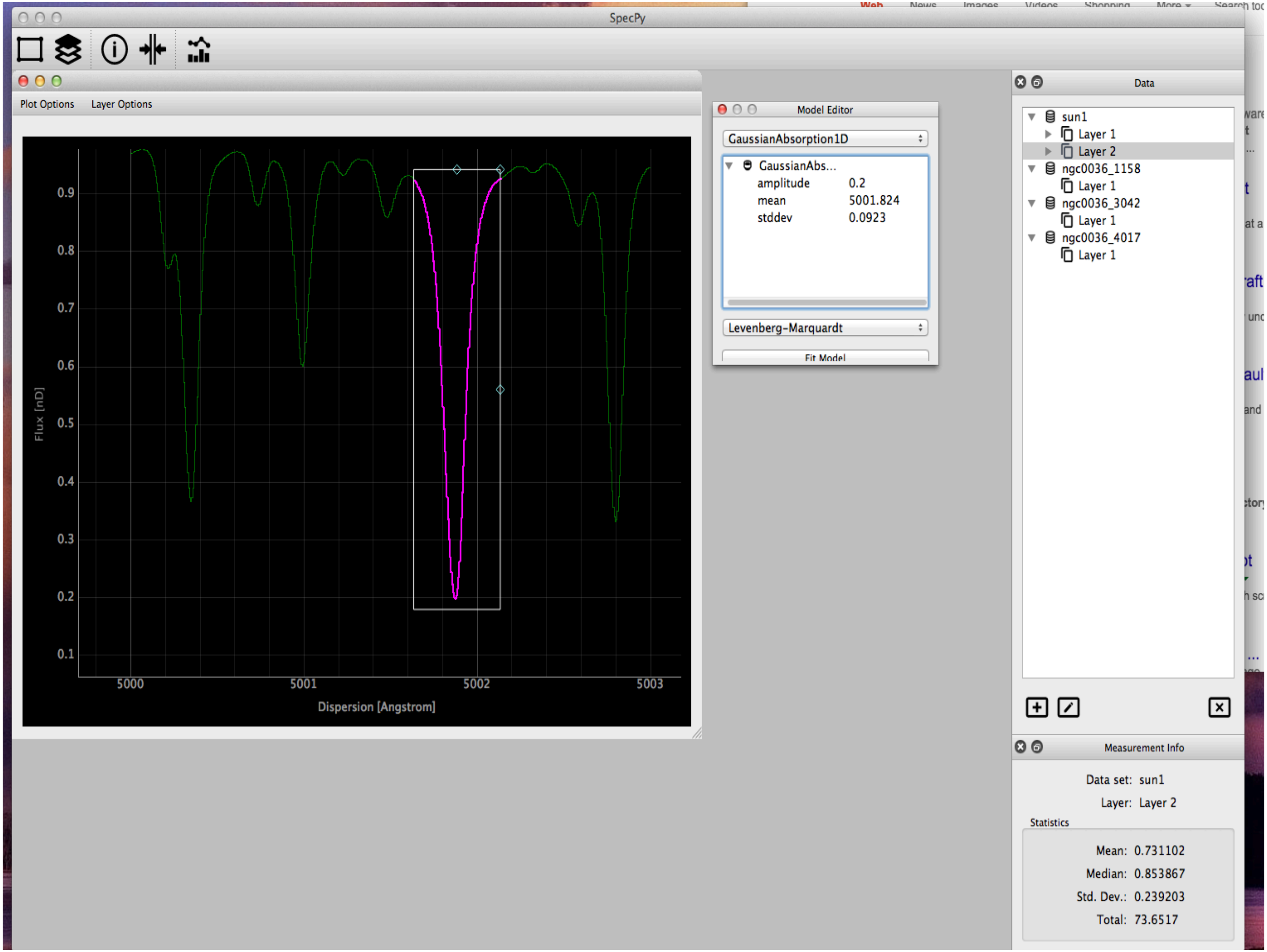


- Visualization tool written in Python developed by Harvard and Chris Beaumont to explore relationships between different representations of data
- We are expecting to use it for MOS visualization and analysis, as well as spectral cube viewing.
- Trying to make it work in different contexts
  - E.g., make it easy to go back an forth from interactive terminal session (or ipython notebook) to the application.
  - Making tools work outside of glue as well as within.

Interactive modeling

Currently working on splot kind of functionality.

- Display multiple overlaid 1-d spectra, model fits, residuals, etc
- Interactions include selecting regions, setting initial parameters (e.g., lines to be fit), etc.
- Separate but coordinating widget to interact with models
  - changing definitions of models
  - adding constraints
    - Upper, lower bounds
    - Equations relating to other parameters, e.g., fixed wavelength ratios.
  - fixing or unfixing parameters
- Keep the basics generic enough to use in other contexts
  - E.g., modeling widget for use in image fitting or WCS fitting
  - 1-d visualization for time series, etc



GaussianAbsorption1D

GaussianAbs...

amplitude	0.2
mean	5001.824
stddev	0.0923

Levenberg-Marquardt

- sun1
  - Layer 1
  - Layer 2
- ngc0036_1158
  - Layer 1
- ngc0036_3042
  - Layer 1
- ngc0036_4017
  - Layer 1

Data set: sun1

Layer: Layer 2

Statistics

Mean:	0.731102
Median:	0.853867
Std. Dev.:	0.239203
Total:	73.6517

Engaging Users in Development

- STScI using "sprints" to try to engage staff astronomers in helping define data analysis tools.
- 3 2-week sprints held so far with 2 per month or so planned.
- Using Trello as a means of floating tasks and features that should be considered as part of a sprint.
- Not sprints in the usual software sense, but still very useful to get feedback
  - Essentially commits an astronomer to be available for helping prioritize features and define user interfaces.
- Not clear if it can be sustained.

Engaging Users (cont.)

- I think it is necessary to involve individuals outside STScI to make this work.
- In other words, make user involvement astropy-wide.
- We welcome others that are interested in providing input on priorities, use cases, user testing (and even code!)
- What is the best way of interacting with the community on when we want info?
  - Mailing list?

Random Observations

- Ignorance is good (in some contexts)
- Do not over-analyze or over-design software
  - Much better to implement and redesign than try to get everything right the first time.
- Worse is better (!?) Google it
- Don't force Python on those not open to trying it!