Advanced Sherpa

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CIAO Workshop
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Opening new vistas with

Advanced Sherpa

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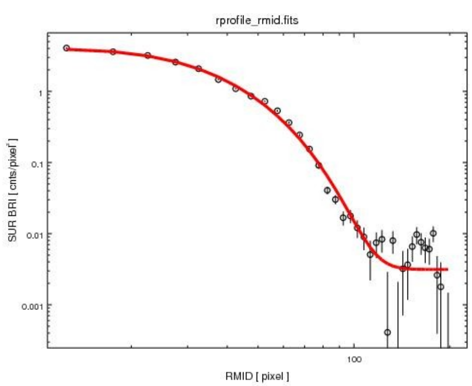
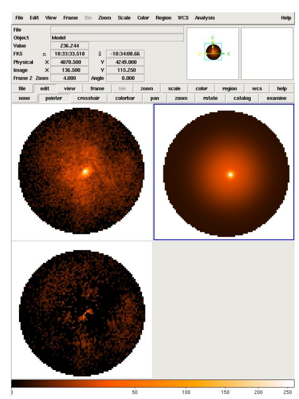
Sherpa

Generalized fitting package with a powerful model language to fit 1D and 2D data

Basic Sherpa

- Interactive (command line) usage
- Scripting using command syntax
- Data access with `show_*` and `print`





```
sherpa> load_pha('acis_pha3.fits')
sherpa> set_source(xsphabs.abs1 * powlaw1d.p1)
sherpa> subtract()
sherpa> fit()
sherpa> show_fit()

Optimization Method: LevMar
name     = levmar
ftol     = 1.19209289551e-07
xtol     = 1.19209289551e-07
gtol     = 1.19209289551e-07
maxfev   = None
epsfcn   = 1.19209289551e-07
factor   = 100.0
verbose = 0

Statistic: Chi2Gehrels

Fit:Dataset               = 1
Method                 = levmar
Statistic              = chi2gehrels
Initial fit statistic = 6.83386e+10
Final fit statistic   = 37.9079 at evaluation 22
Data points            = 44
Degrees of freedom     = 42
Probability [Q-value] = 0.651155
Reduced statistic      = 0.902569
Change in statistic    = 6.83386e+10
   p1.gamma       2.15852
   p1.ampl        0.00022484
```

This works very well much of the time, but ...

Doing more with Sherpa

Python Inside: Sherpa user interface and high-level functions are Python

- Sherpa provides an interface to let users:
  - Access the internal objects used within Sherpa
  - Easily define user model and user statistic functions
  - Use Sherpa as an imported library in your Python program
- Paradigm change – CIAO/Sherpa is not the environment, it is a powerful library tool in your Python analysis environment[1].
- Move beyond short *scripts* to full-blown *programs*[2].
- Real life examples:
  - Fit X-ray models to hundreds of Chandra L3 sources (including faint ones), put results in a database, and import to a google web app to browse the results.
  - Fit data where the errors are dominated by quantization (i.e. data are integerized)
  - Generate complex thermal models requiring parallel fitting using > 30 CPUs and a GUI fitting application

[1]Sherpa can even run outside of CIAO! See http://cxc.cfa.harvard.edu/contrib/sherpa/

[2]See http://www.astropython.org and http://python4astronomers.github.com for more about Python and astronomy

Topics

Take another swig of coffee and get ready for some code

- Getting data into Sherpa
- Digging into Sherpa: getting at the objects underneath
- Creating user models and user statistics functions
  - Using functions
  - Using classes (you too can write an OOP)
- Goodness of fit for low-count X-ray spectra
- Parallelization with MPI

Sit back and relax

- Deproject: a Sherpa extension module
- Keeping Chandra cool: a Sherpa success story

Getting data into Sherpa

- Sherpa has many ways of loading data and other things:

```
sherpa-17> load_<TAB>
load_arf              load_bkg_arf     load_filter      load_pha          load_state        load_user_model
load_arrays           load_bkg_rmf     load_grouping    load_preferences  load_staterror    load_user_stat
load_ascii            load_colormap    load_image       load_psf          load_syserror
load_ascii_transform  load_conv        load_multi_arfs  load_quality      load_table
load_bkg              load_data        load_multi_rmfs  load_rmf          load_table_model
```

- One of my favorites doesn't appear in any Sherpa thread[1] : `load_arrays()`
- This provides a generic way to load *memory arrays* as Sherpa datasets
- Example: ASCII file format not understood by Sherpa. Instead use asciitable[2]

```
sherpa> load_data('csc.rdb[cols ra, dec]')
IOErr: opening file  has failed with ERROR - Failed to open 'csc.rdb[cols ra, dec]'.

sherpa> import asciitable
sherpa> dat = asciitable.read('csc.rdb', Reader=asciitable.RdbReader)
sherpa> load_arrays(1, dat['ra'], dat['dec'], Data1D)
```

[1] From the google search “sherpa load_arrays”
[2] http://cxc.harvard.edu/contrib/asciitable

Sherpa

Getting data into Sherpa

- Didn't we just replace one line with three? But now we **own** the data!

```
sherpa> dat = asciitable.read('csc.rdb')
sherpa> ra = dat['ra']
sherpa> dec = dat'dec']
Sherpa> dist = calc_dist(ra, dec, ra.mean(), dec.mean())
sherpa> load_arrays(1, dist, dat['mag'], Data1D)
```

- `load_arrays()` works for 2-D and PHA data as well

HINT: get help on CIAO functions by googling “ahelp <function>” or “ciao ahelp <function>”. This doesn't seem to work with bing.

Digging into Sherpa: getting the good bits

- Sherpa also has many ways of showing the current analysis state:

```
sherpa> show_<TAB>
show_all show_bkg_model  show_conf  show_data   show_fit    show_method show_proj show_source
show_bkg show_bkg_source show_covar show_filter show_kernel show_model  show_psf  show_stat
```

```
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sherpa> subtract()
sherpa> fit()
Sherpa> show_fit()
Optimization Method: LevMar
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ftol    = 1.19209289551e-07
xtol    = 1.19209289551e-07
gtol    = 1.19209289551e-07
maxfev  = None
epsfcn  = 1.19209289551e-07
factor  = 100.0
verbose = 0

Statistic: Chi2Gehrels
Chi Squared with Gehrels variance

Fit:Dataset               = 1
Method                 = levmar
Statistic              = chi2gehrels
Initial fit statistic = 31.5124
Final fit statistic    = 31.5124 at evaluation 5
Data points            = 1024
Degrees of freedom     = 1021
Probability [Q-value] = 1
Reduced statistic      = 0.0308642
Change in statistic    = 8.81487e-07
   abs1.nH        0.112892
   p1.gamma       3.07627
   p1.ampl        0.00011212
```

- Great for interactive analysis but what about *using* the results?
- OLD school
  - Run as a script and pipe output to a file
  - Write a separate script (perl?) to parse and store in a new table
  - Writing code to reliably parse all these tidbits is a very fun and interesting way to spend your day. NOT.
- Nice shiny way
  - Run as a python script
  - Directly access results and store in desired format .. or use python twitter API to immediately tweet the results.

Digging into Sherpa: getting the good bits

- Sherpa lets you `get_*` what you need:

```
sherpa> get_<TAB>
Display all 188 possibilities? (y or n)
get_analysis             get_contour_levels       get_fit_plot             get_model_plot           get_psf_plot
get_areascal             get_contour_range        get_fit_results          get_model_plot_prefs     get_pyType
get_arf                  get_contour_visible      get_frame                get_model_type           get_quality
get_arf_plot             get_contour_xrange       get_frame_border_visible get_num_par              get_rate
get_attribute            get_contour_yrange       get_frame_scale          get_num_par_frozen       get_ratio_contour
get_axes                 get_contour_zrange       get_frame_visible        get_num_par_thawed       get_ratio_image
get_axis                 get_coord                get_functions            get_number_cols          get_ratio_plot
get_axis_range           get_counts               get_grouping             get_number_rows          get_reg_proj
get_axis_scale           get_covar                get_histogram            get_object_coordinfo     get_reg_unc
get_axis_text            get_covar_opt            get_histogram_range      get_object_count         get_region
get_axis_transform       get_covar_results        get_histogram_xrange     get_order_plot           get_region_visible
get_axis_visible         get_covariance_results   get_histogram_yrange     get_par                  get_resid_contour
get_backscal             get_crate_item_type      get_image                get_photon_flux_hist     get_resid_image
get_bkg                  get_crate_type           get_image_range          get_pick                 get_resid_plot
get_bkg_arf              get_curve                get_image_visible        get_pileup_model         get_rmf
get_bkg_chisqr_plot      get_curve_range          get_image_xrange         get_piximg               get_server_id
get_bkg_delchi_plot      get_curve_visible        get_image_yrange         get_piximg_shape         get_source
get_bkg_fit_plot         get_curve_xrange         get_indep                get_piximgvals           get_source_contour
get_bkg_model            get_curve_yrange         get_int_proj             get_plot                 get_source_image
get_bkg_model_plot       get_data                 get_int_unc              get_plot_aspect_height   get_source_plot
get_bkg_plot             get_data_aspect_ratio    get_kernel_contour       get_plot_aspect_ratio    get_specresp
get_bkg_ratio_plot       get_data_contour         get_kernel_image         get_plot_aspect_width    get_split_plot
get_bkg_resid_plot       get_data_contour_prefs   get_kernel_plot          get_plot_range           get_stat
get_bkg_rmf              get_data_image           get_key                  get_plot_title           get_stat_name
get_bkg_source           get_data_plot            get_key_names            get_plot_visible         get_staterror
get_bkg_source_plot      get_data_plot_prefs      get_keyval               get_plot_xrange          get_syserror
get_chisqr_plot          get_default_depth        get_label                get_plot_yrange          get_transform
get_col                  get_default_id           get_label_text           get_point
get_transform_matrix
get_col_names            get_delchi_plot          get_line                 get_point_visible        get_transform_type
get_colorbar             get_dep                  get_method               get_preference           get_window
get_colorbar_border_visible get_dims              get_method_name          get_preferences          get_window_title
get_colorbar_visible     get_dmType               get_method_opt           get_proj                 get_xaxis
get_colvals              get_dmType_str           get_model                get_proj_opt             get_xsabund
get_conf                 get_energy_flux_hist     get_model_autoassign_func get_proj_results        get_xscosmo
get_conf_opt             get_error                get_model_contour        get_projection_results   get_xsxsect
get_conf_results         get_exposure             get_model_contour_prefs  get_psf                  get_yaxis
get_confidence_results   get_filter               get_model_image          get_psf_contour
get_contour              get_fit_contour          get_model_pars           get_psf_image
```

Digging into Sherpa: getting the good bits

- Most everything you get_*() will be a python object and that's the prize
  - Internally Sherpa uses hierarchical objects for most things
  - You can find and examine internal object attributes by <TAB> digging

```
sherpa> load_pha(1, 'acis_pha3.fits')
sherpa> dataset = get_data(1)
sherpa> dataset
        <DataPHA data set instance 'acis_pha3.fits'>
sherpa> dataset.<TAB>
Display all 159 possibilities? (y or n) n

sherpa> dataset.get_<TAB>
...
sherpa> counts = dataset.counts
sherpa> b = numpy.where(dataset.counts > 3)
sherpa> b
        (array([ 14,  16,  30,  45,  97, 118]),)
sherpa> c = dataset.channel[b]
sherpa> e = dataset._channel_to_energy(c)
array([ 0.2117,  0.2409,  0.4453,  0.6643,  1.4235, 1.7
```

numpy: core python numerical library
where(): return indices where expr is True

Return selected elements from channel array

I found this function just by <TAB> digging.
The _ in front means it wasn't intended for external use but why not live dangerously.
Documentation? Who needs it.

- With some care you can manipulate the internal object attributes

```
sherpa> dat = asciitable.read('csc.rdb', Reader=asciitable.RdbReader)
sherpa> load_arrays(1, dat['ra'], dat['dec'], Data1D)
sherpa> dataset = get_data()
sherpa> dataset.y = dataset.x**2
sherpa> dataset.staterror = dataset.y / 20
```

Digging into Sherpa: source and fit results

- Now something more useful: examine source model parameters and fit results

```
sherpa> source = get_source()
sherpa> source.parts
(<XSphabs model instance 'xsphabs.abs1'>,
 <PowLaw1D model instance 'powlaw1d.p1'>)

sherpa> for par in source.pars:
             print par.fullname, par.val, par.min, par.max, par.frozen

abs1.nH 0.112891604641 0.0 100000.0 False
p1.gamma 3.0762703235 -10.0 10.0 False
p1.ref 1.0 -3.40282346639e+38 3.40282346639e+38 True
p1.ampl 0.000112120110443 0.0 3.40282346639e+38 False

sherpa> fit = get_fit_results()
sherpa> print [x for x in dir(fit) if not x.startswith('_')]
['covarerr', 'datasets', 'dof', 'dstatval', 'extra_output', 'format', 'istatval',
'message', 'methodname',
 'modelvals', 'nfev', 'numpoints', 'parnames', 'parvals', 'qval', 'rstat', 'statname',
'statval', 'succeeded']
```

Digging into Sherpa: source and fit results

- Don't just examine. ***Organize*** and tabulate!

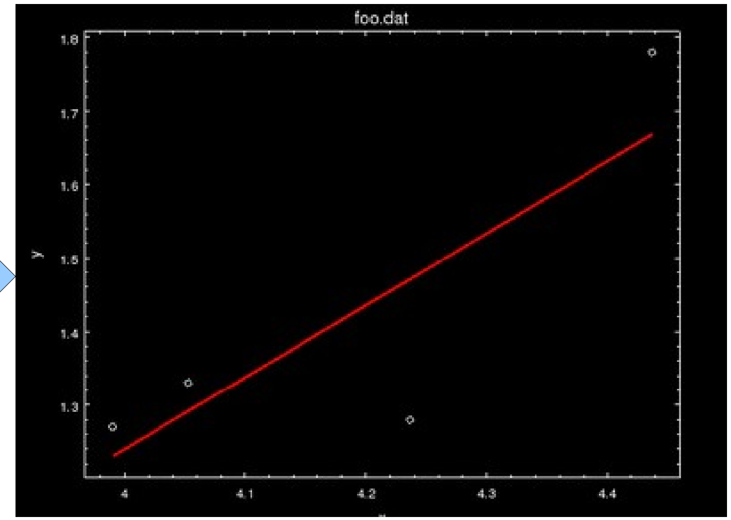
```
import sqlite3
conn = sqlite3.connect('csc_fits.db')
c = conn.cursor()
c.execute("""create table fit_pars
 (source_name text, par_name text, par_val real)""")

for parname, parval in zip(fit.parnames, fit.parvals):
    c.execute("insert into fit_pars values (?, ?, ?)",
              (source.name, parname, parval))

conn.commit()
c.close()
```

```
ccosmos% sqlite3 csc_fits.db
SQLite version 3.3.6
Enter ".help" for instructions
sqlite> select * from fit_pars;
(xsphabs.abs1 * powlaw1d.p1)|abs1.nH|0.112891604640818
(xsphabs.abs1 * powlaw1d.p1)|p1.gamma|3.07627032349591
(xsphabs.abs1 * powlaw1d.p1)|p1.ampl|0.000112120110443 43
```

User models with python functions

- Adding a user model defined with a python function is *shockingly simple!*

```
def myline(pars, x):
    return pars[0] * x + pars[1]

load_user_model(myline, "myl")
add_user_pars("myl", ["m","b"])
set_source(myl)

myl.m=30
myl.b=20
```



Sure, but any real model has to be written in C or Fortran, right? Not necessarily.

- Numerical processing with **NumPy** is in C so any vectorized calculations are fast.
- The **SciPy** library provides a large selection of optimized numerical algorithms using well known fortran and C numerical libraries.
- Prototype the user model in Python. If it's too slow then profile the code and convert the hot spots to C or C++.

But what about my existing C / Fortran model code? Google "sherpa user models".

Sherpa

User models with Python classes

- Frequently a user model function requires associated metadata (atomic data, table file names, non-fitted parameters, etc)
- This is a typical problem in fitting (remember Fortran COMMON blocks?)
- Python provides a very clean solution: **classes**

Ever wonder what's the deal with "object oriented programming"? Here it is. The object stores metadata.

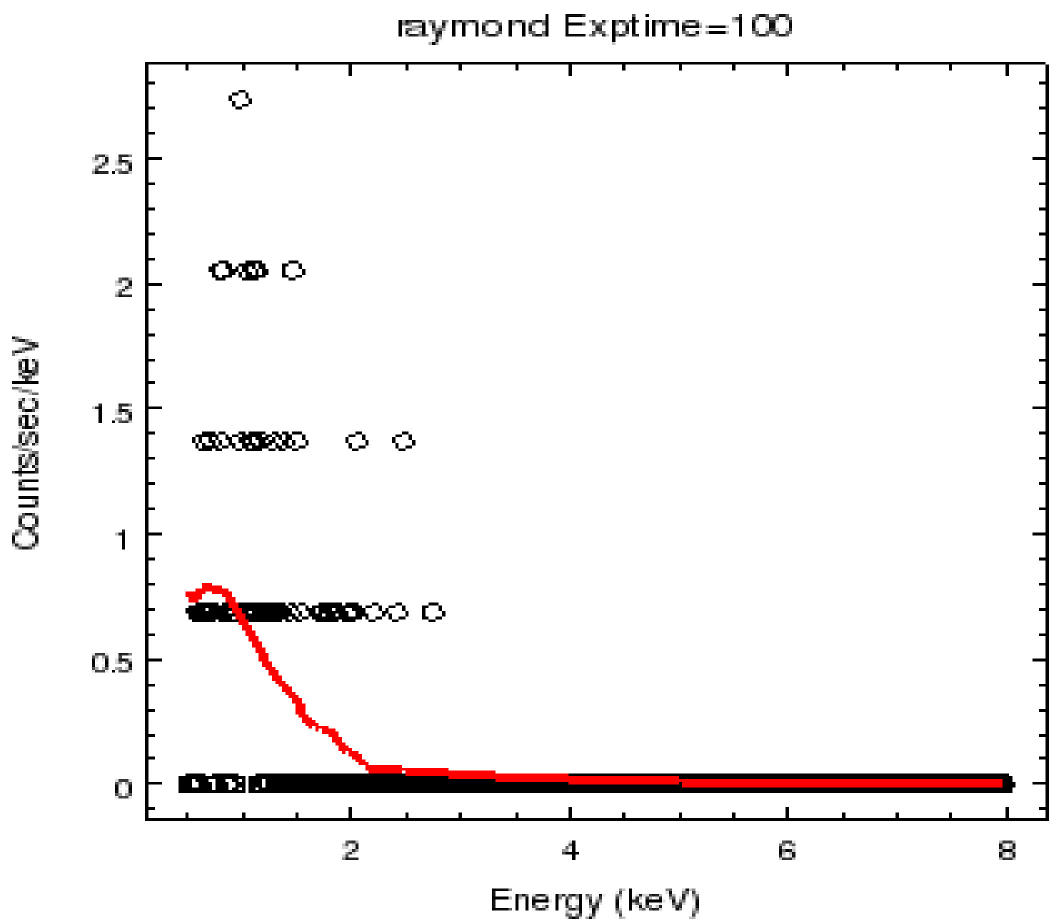
```
class FITS_TableModel(object):
    """Simplest possible FITS table model.  Table has two col
        kT       : temperature
        spectrum : corresponding spectrum in an N-element array
       In this model the spectrum nearest in temperature is returned.
       The energy bins of the fitted spectrum is ignored here.
    """
    def __init__(self, filename):
        hdus = pyfits.open(filename)
        self.kT = hdus[1].data.field('kT')
        self.spectra = hdus[1].data.field('spectrum')
        hdus.close()

    def __call__(self, pars, x):
        kT = pars[0]
        i = numpy.searchsorted(self.kT, [kT])[0]
        if (kT - self.kT[i-1]) < (self.kT[i] - kT):
            i -= 1
        return self.spectra[i]

user_model_func = FITS_TableModel('plasma_spectra.fits')
load_user_model(user_model_func,"myspec")
add_user_pars("myspec", ["kT"])
set_source(myspec)
```

Object initialization with "filename" via __init__. Read the FITS data and store within the object.

Here's the magic: the object created by the class can be called directly as a function and it will run the special __call__ method.

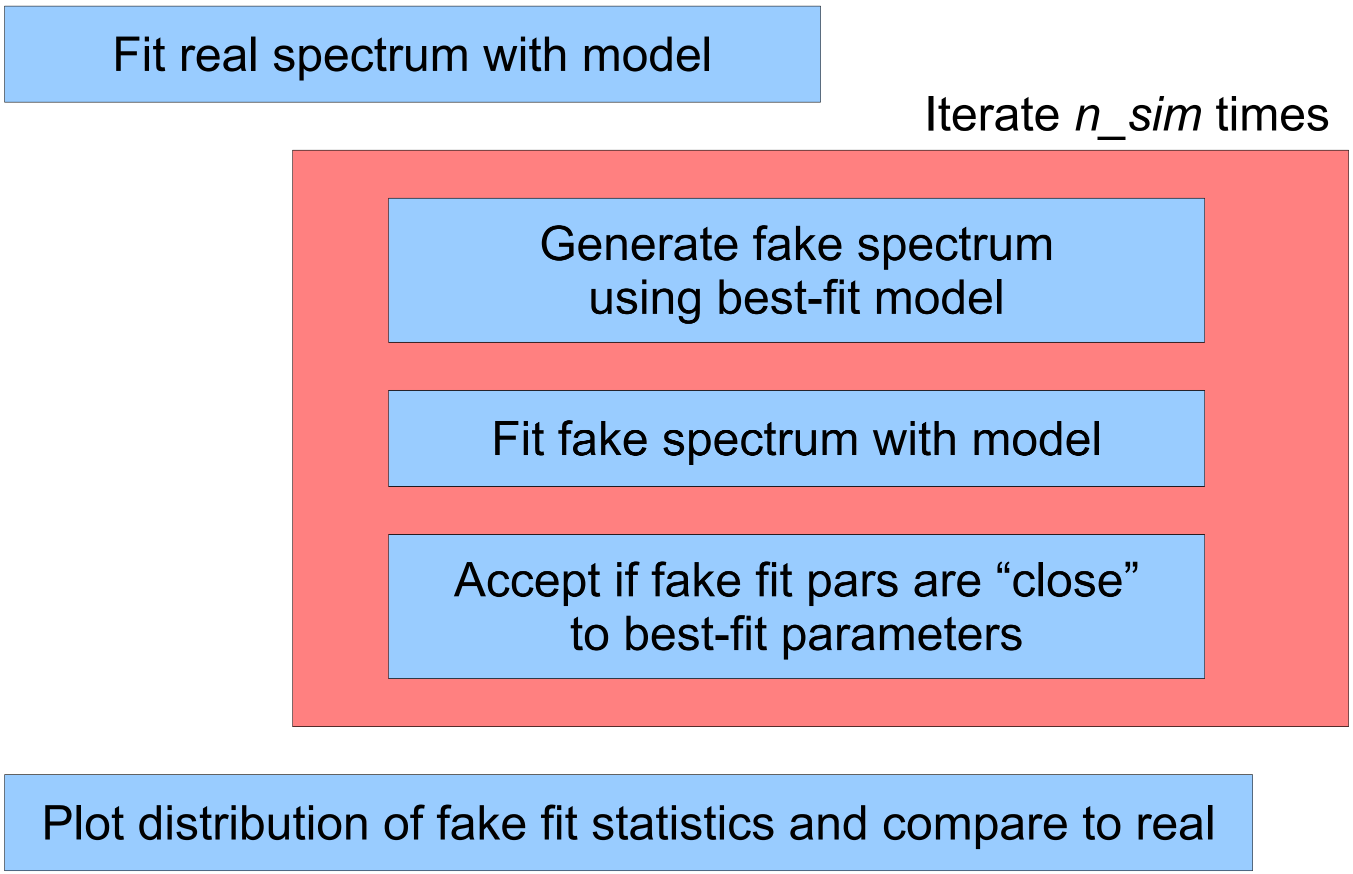
Goodness of fit by simulation

- Measuring the *goodness of fit* is challenging for low-count spectra
  - “Is the X-ray emission thermal or non-thermal (power-law)?”
  - Cannot easily eye-ball the data and model fit
  - No simple analogs to reduced Chi^2 distribution for Cash (likelihood) statistic
  - Challenging, but not impossible, and worth the trouble



Goodness of fit by simulation

- Simulation provides a way to estimate whether the observed fit statistic would be unusual for an ensemble of data realizations of the source model[1].



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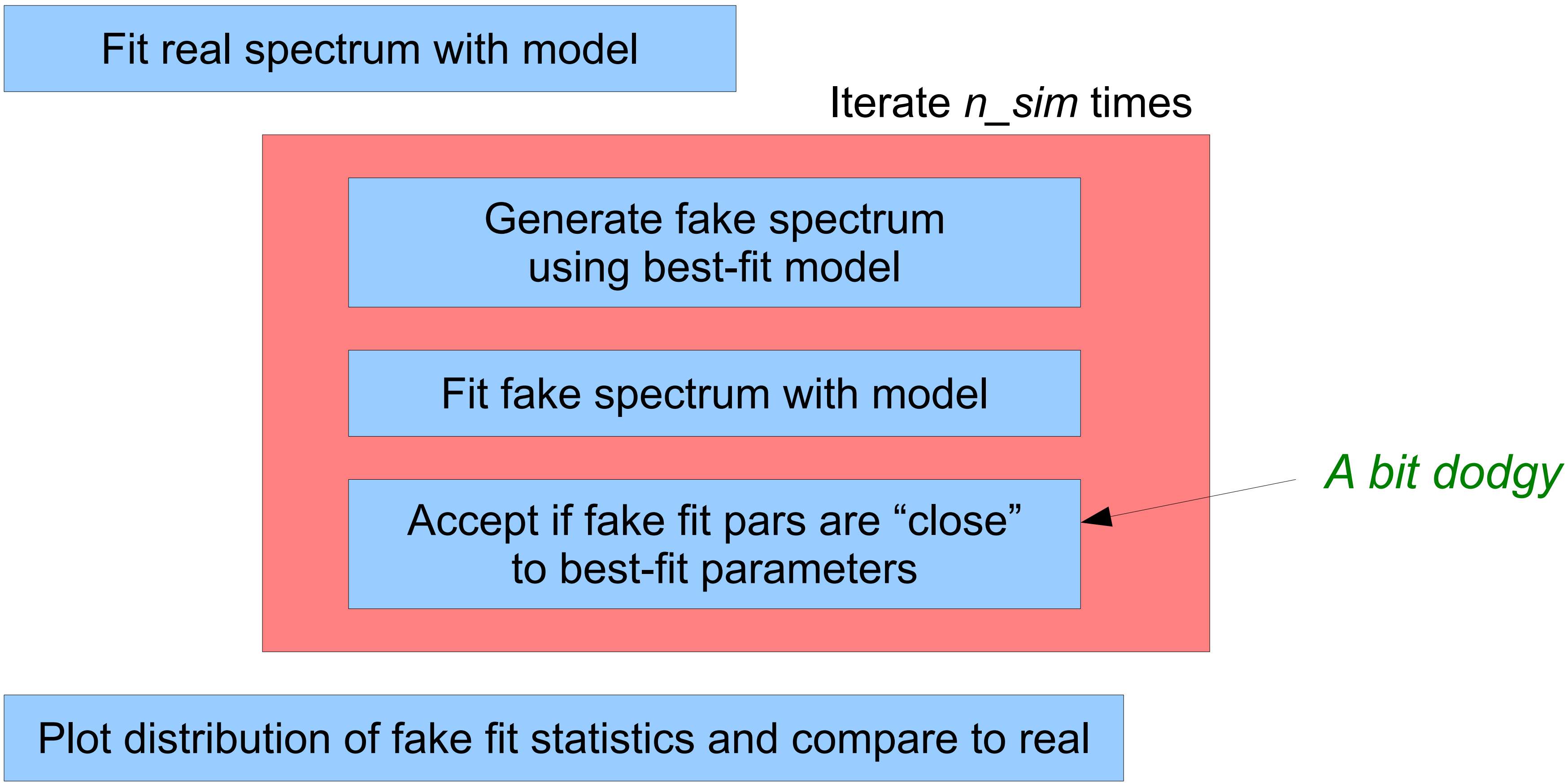


[1] *Warning: this algorithm is not statistician-approved and needs more testing.*

Sherpa

Goodness of fit by simulation

Model selection simulation:

- Generate a spectrum using a Raymond-Smith source model.
- Try to decide if a power-law model is consistent with the spectrum

```
import numpy as np

n_sim = 2000
exposure0 = 200
spectype = 'raymond'

# Generate the simulated "real" data (Raymond-Smith plasma kT=1.5 keV)
set_source(1, "xsraymond.ray1")
ray1.kt = 1.5
ray1.norm = 3e-3
arf = unpack_arf('acis7s.arf')
rmf = unpack_rmf('acis7s.rmf')
fake_pha(1, arf=arf, rmf=rmf, exposure=exposure0)

notice(0.5, 8)
set_method('levmar')
set_stat('cash')
```

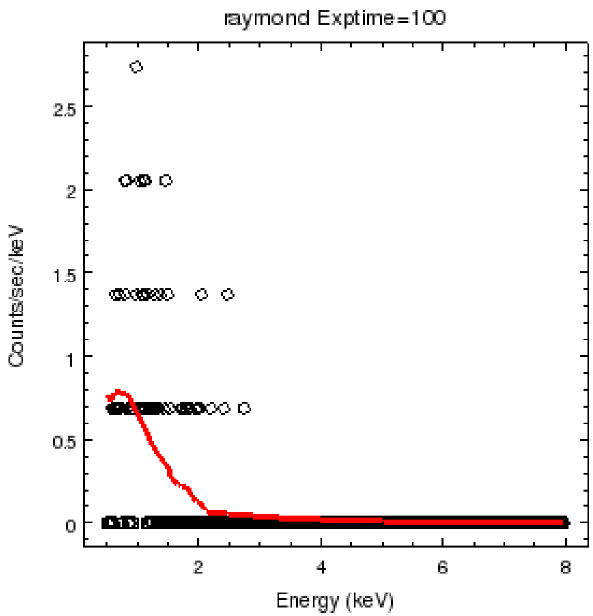
Goodness of fit by simulation

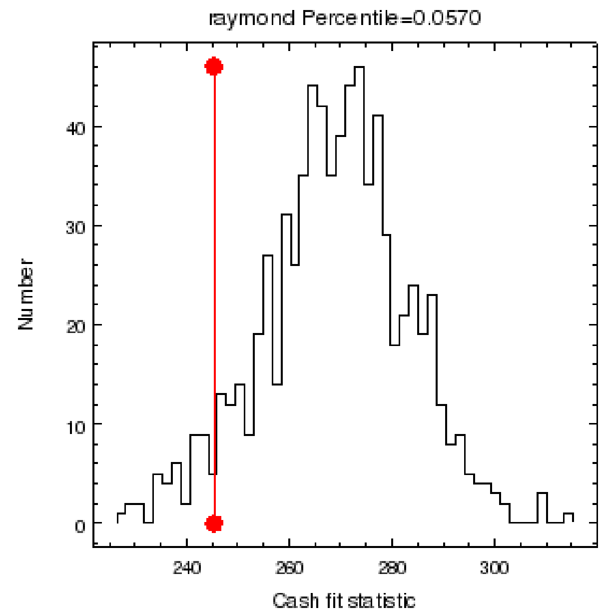
```
# Model this spectrum with an unabsorbed power law
set_source(1, "powlaw1d.pow1")
fit()
gamma0 = pow1.gamma.val
ampl0 = pow1.ampl.val

# Store results from initial fit of “real” data
fit_results = get_fit_results()
stat0 = fit_results.statval
flux0 = calc_energy_flux(lo=0.5, hi=8.0)

stats = np.zeros(n_sim)
gammas = np.zeros(n_sim)

for i in range(n_sim):
    # Reset parameter values to best fit and generate fake spectrum
    pow1.gamma = gamma0
    pow1.ampl = ampl0
    fake_pha(1, arf=arf, rmf=rmf, exposure=exposure0)

    # Fit and record statistics
    fit()
    stats[i] = calc_stat()
    gammas[i] = pow1.gamma.val
    print i
```

Goodness of fit by simulation

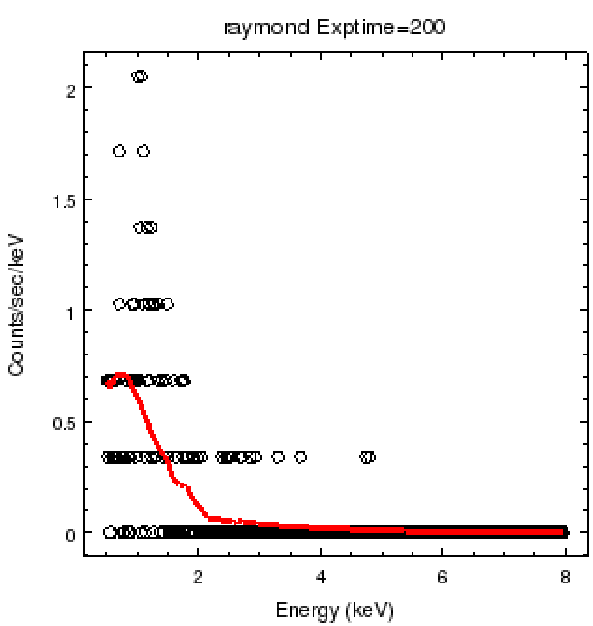
```
# Select the simulations that were "close" to the best-fit gamma
ok = (gammas > gamma0 - 0.1) & (gammas < gamma0 + 0.1)
stats = np.sort(stats[ok])

# Sort the statistics in order and rank the fit stat from the "real" data
n_stats = len(stats)
rank = np.searchsorted(stats, stat0)
percentile = float(rank) / n_stats
print 'fit stats (rank, n_stats, percentile) : {0} {1} {2:.4f}'.format(
    rank, n_stats, percentile)

# Make some plots
bin_vals, bin_edges = np.histogram(stats, bins=50)
bin_lefts = bin_edges[:-1]
bin_rights = bin_edges[1:]
add_window()
add_histogram(bin_lefts, bin_rights, bin_vals)

add_curve([stat0, stat0], [0, bin_vals.max()])
set_curve(['symbol.color', 'red',
           'line.color', 'red',
           'symbol.style', 'circle'])
set_plot_title('{0} Percentile={2:.4f}'.format(spectype, exposure0,
percentile))
set_plot_xlabel('Cash fit statistic')
set_plot_ylabel('Number')
print_window('{0}_hist_{1}.png'.format(spectype, exposure0))
```

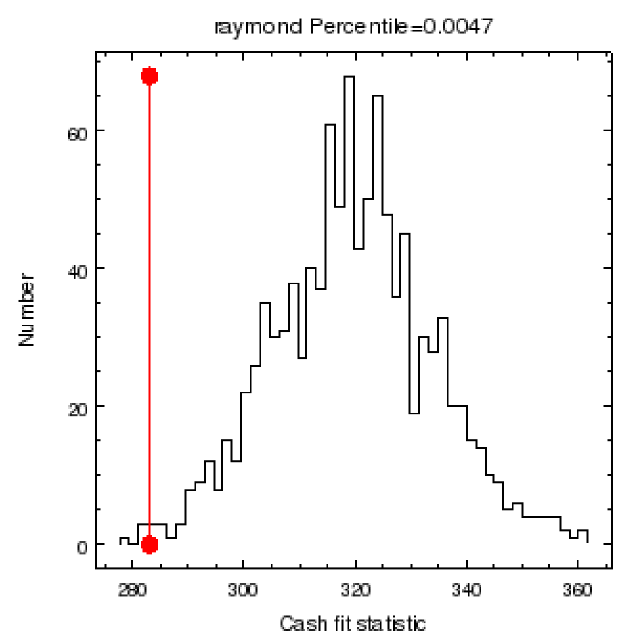
Goodness of fit by simulation





70 counts
Confidence ~0.94



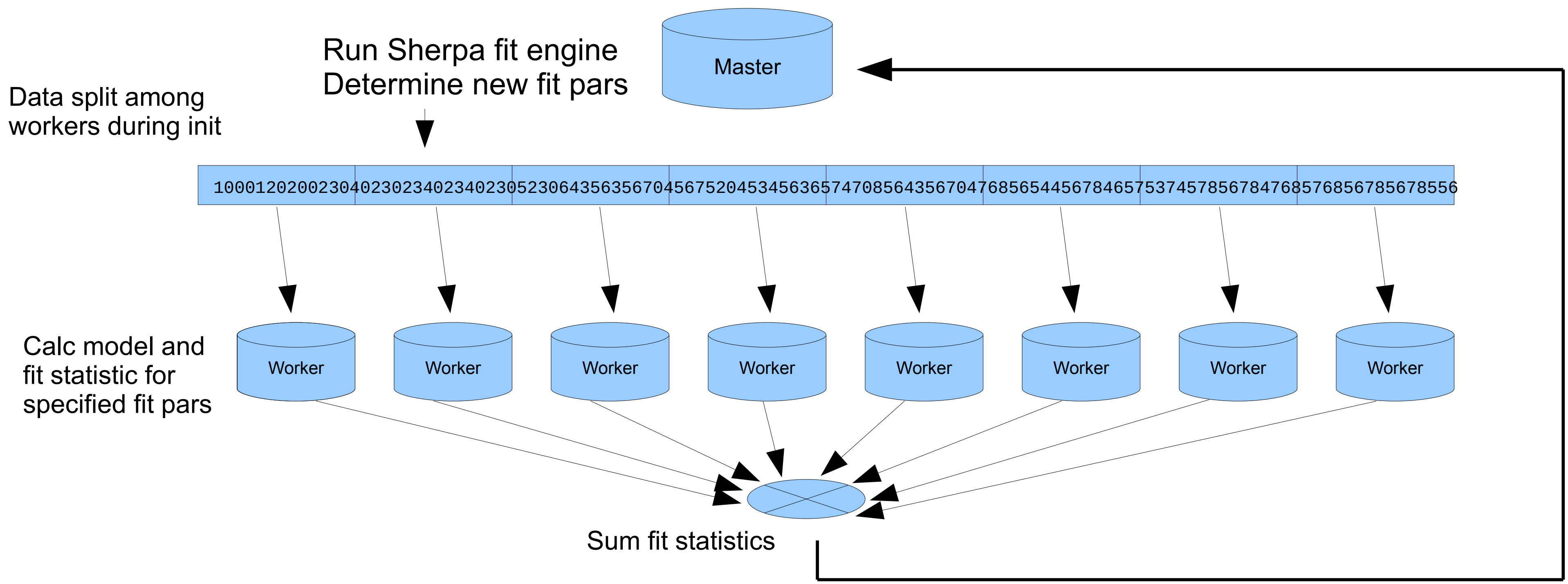


140 counts
Confidence ~0.995

“Power-law model is not a likely source for the spectrum”
(truth =Raymond-Smith kT=1.5)

Parallelization

- For some problems with large datasets or computationally intensive models it may be possible to improve fit performance by using multiple processors.
- Processors can be on the same machine or in a networked cluster.
- Sherpa already takes advantage of multiple cores in projection and conf.
- Improving fit performance is tricky for convolved models but easy for models that can be split in data space[1].



[1]Splitting in data space is just one of many possible strategies

Parallelization with MPI

- Can do parallel processing using C and Python implementations of the widely used Message Passing Interface standard.

```
class CalcModel(object):
    def __init__(self, x, y):
        msg = {'cmd': 'init', 'x': x, 'y': y}
        comm.bcast(msg, root=MPI.ROOT)

    def __call__(self, pars, x):
        comm.bcast(msg={'cmd': 'calc_model', 'par': par}, root=MPI.ROOT)
        return numpy.ones_like(x)    # Dummy value of correct length

def calc_staterror(data):
    return numpy.ones_like(data)

class CalcStat(object):
    def __call__(self, data, model, staterror=None, syserror=None, weight=None):
        msg = {'cmd': 'calc_statistic'}
        comm.bcast(msg, root=MPI.ROOT)
        fit_stat = numpy.array(0.0, 'd')
        comm.Reduce(None, [fit_stat, MPI.DOUBLE], op=MPI.SUM, root=MPI.ROOT)
        return fit_stat.tolist(), numpy.ones_like(data)

comm = MPI.COMM_SELF.Spawn(sys.executable, args=['fit_worker.py'], maxprocs=nproc)
load_arrays(1, x, y)
load_user_model(CalcModel(x, y), 'mpimod')
add_user_pars('mpimod', parnames)
set_model(1, mpimod)
load_user_stat('mpistat', CalcStat(), calc_staterror)
set_stat(mpistat)
fit(1)
```

Parallelization with MPI

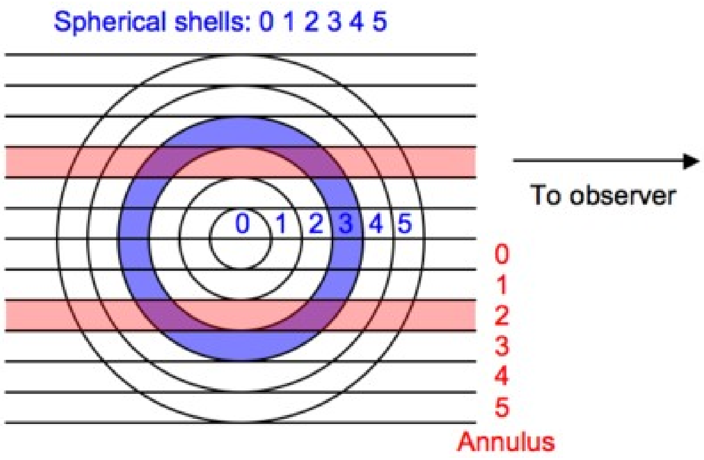
The fit_worker code just waits around to get instructions.

```
def calc_model(pars, x):
    # calculate the model values
    return model

comm = MPI.Comm.Get_parent()
size = comm.Get_size()
rank = comm.Get_rank()

while True:
    msg = comm.bcast(None, root=0)

    if msg['cmd'] == 'stop':
        break

    elif msg['cmd'] == 'init':
        i = numpy.int32(numpy.linspace(0.0, len(msg['x'], size+1))
        i0 = i[rank]
        i1 = i[rank+1]
        data_x = msg['x'][i0:i1]
        data_y = msg['y'][i0:i1]

    elif msg['cmd'] == 'calc_model':
        model = calc_model(msg['pars'], data_x)

    elif msg['cmd'] == 'calc_statistic':
        fit_stat = numpy.sum((data_y - model)**2)
        comm.Reduce([fit_stat, MPI.DOUBLE], None, op=MPI.SUM, root=0)

comm.Disconnect()
```

Deproject: a Sherpa extension module

Deproject is a CIAO Sherpa extension package to facilitate deprojection of two-dimensional annular X-ray spectra to recover the three-dimensional source properties.

- The deproject module creates a framework for manipulation of a stack of related input datasets and their models.
- Most of the functions resemble ordinary Sherpa commands (e.g. set_par, set_source, ignore) but operate on a stack of spectra.

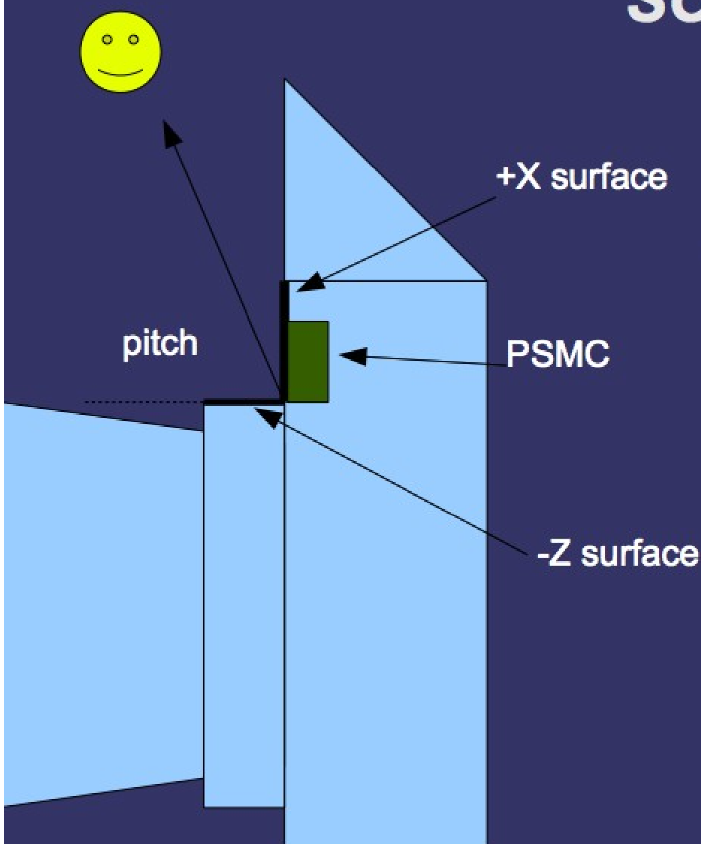


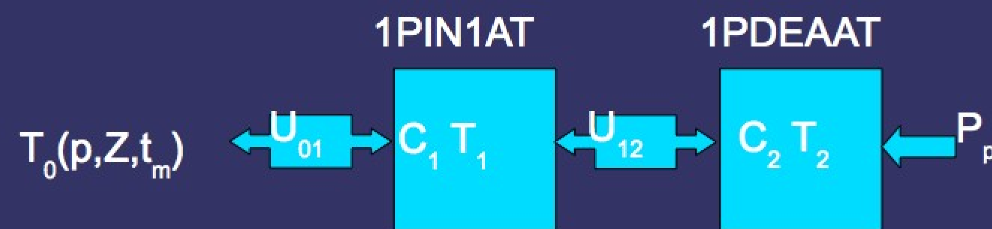
Keeping Chandra cool: a Sherpa success story

Keeping Chandra cool: a Sherpa success story

Keeping Chandra cool: a Sherpa success story

SOT PSMC model



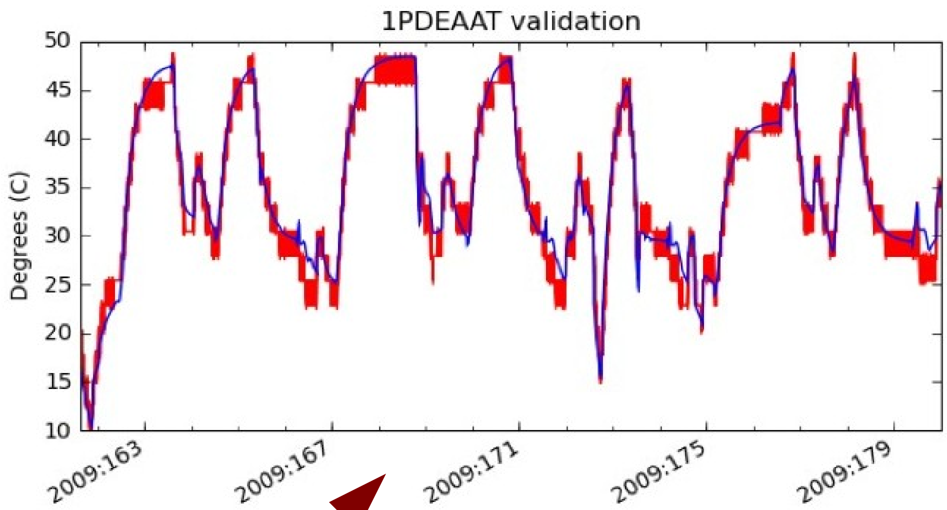


$$C_1 \frac{dT_1}{dt} = U_{01}(T_0 - T_1) + U_{12}(T_2 - T_1)$$

$$C_2 \frac{dT_2}{dt} = P_p + U_{12}(T_1 - T_2)$$

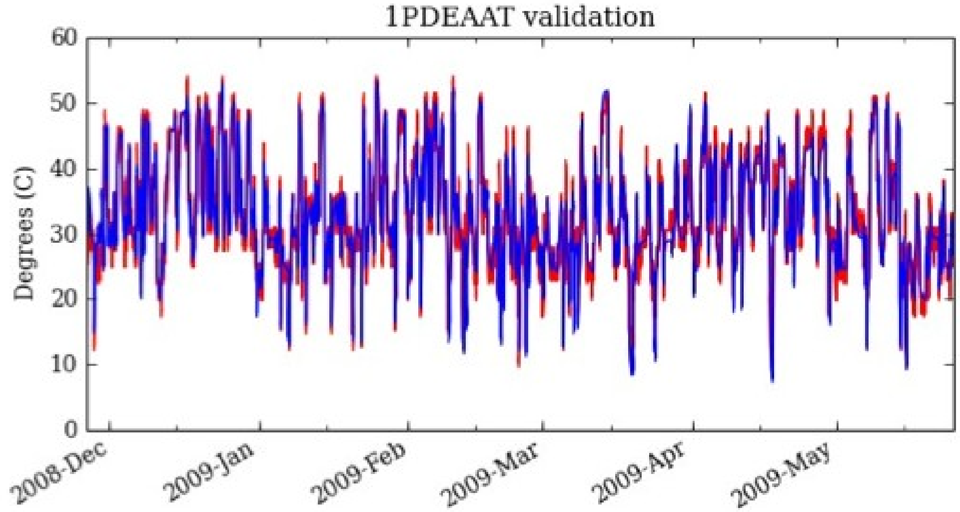
- Key inputs to model are pitch angle, SIM-Z position and ACIS power.
- Total of 13 model coefficients.

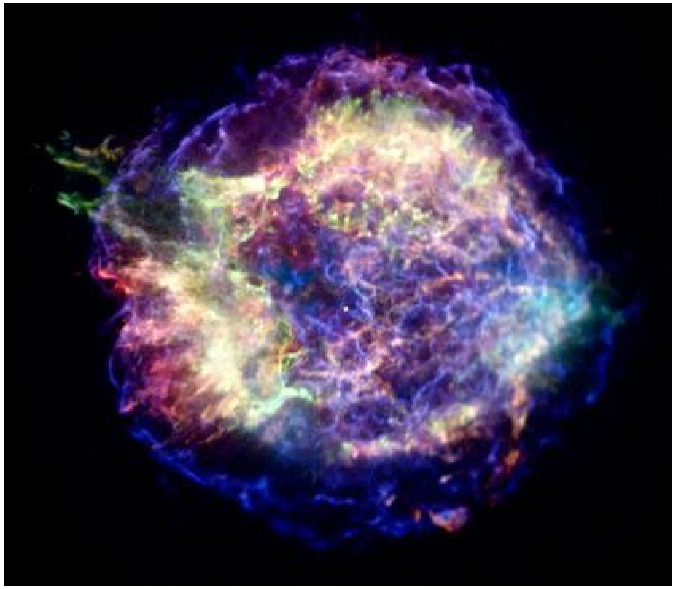
Keeping Chandra cool: a Sherpa success story



Predictions for mission planning

Calibration: Sherpa





Conclusions

- Sherpa provides next-generation capability through Python scripting
- Your time investment to learn Sherpa will pay off
- Learn Python!
  - http://python4astronomers.github.com
  - Python + analytic skills = Job security