Introduction to Sherpa

Aneta Siemiginowska

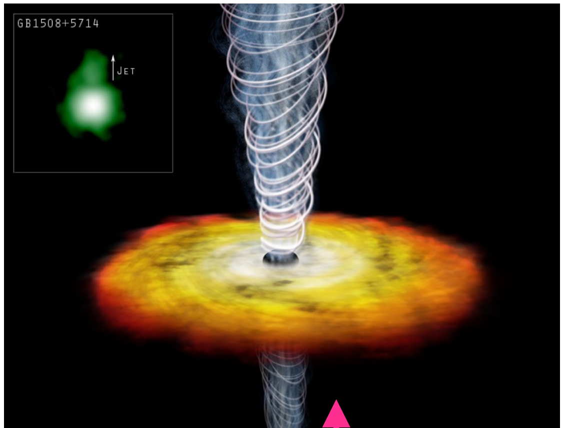
Chandra X-ray Center

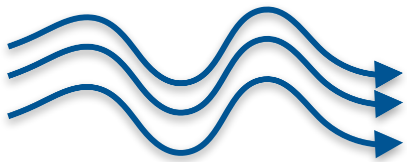
http://cxc.harvard.edu/sherpa

CIAO Workshop NCRA - Pune - October 2017

Observations and Data Collection

Astrophysical process



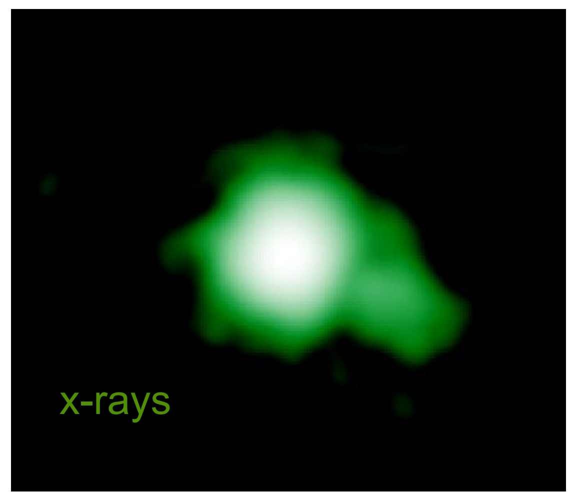


Random number of photons reach the detector

?

draw conclusion about the astrophysical source

Detector collects photons, adds noise



Scientific Experiment

Observations

Data Preparation

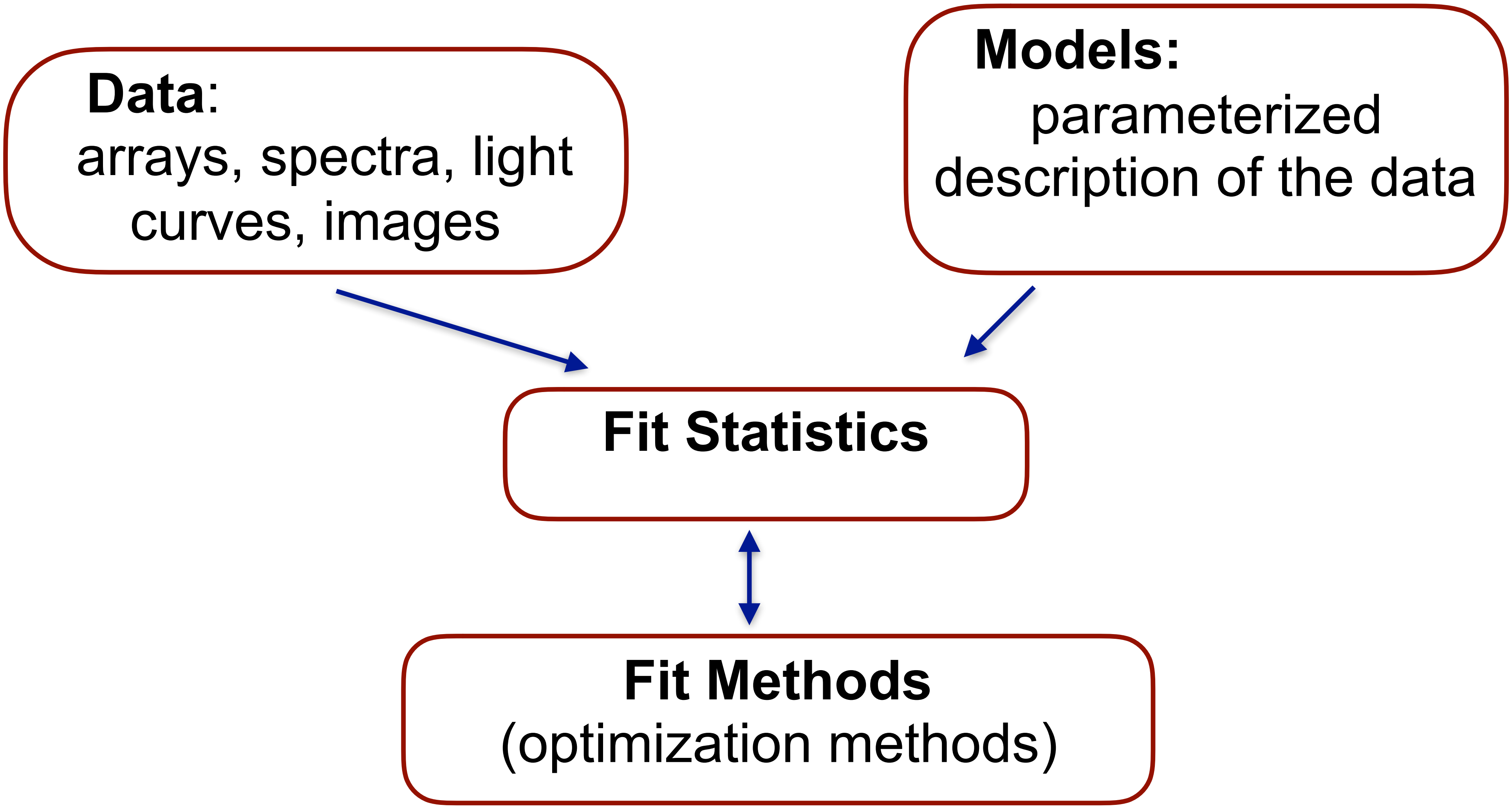
Instrument specific processing software such as CIAO

Data Analysis:
source detections, source properties,
image analysis, features, spectra, physical properties of the source, ***apply models*** to understand the source nature

Conclusions and Final Decision

Sherpa

Sherpa



Sherpa

Data Input/Output
Astropy.io
PyCrates

Models Library
Sherpa, XSPEC models,
user models, templates

Fit Statistics: Poisson and Gaussian likelihood

Fit Methods:
minimization and sampling

Visualization:
ChIPS, ds9, matplotlib

Final Evaluation
& Conclusions

Data in Sherpa

- X-ray Spectra
  typically PHA files with the RMF/ARF calibration files
- X-ray Images
  FITS images, exposure maps, PSF files
- Lightcurves
  FITS tables, ASCII files
- Derived functional description of the source:
  - Radial profile
  - Temperatures of stars
  - Source fluxes
- Concepts of Source and Background data
- Any data array that needs to be fit with a model

Data in Sherpa

- Load functions to input data:

  data: load_data, load_pha, load_arrays, load_ascii
  calibration: load_arf, load_rmf load_multi_arfs, load_multi_rmfs
  background: load_bkg, load_bkg_arf , load_bkg_rmf
  2D image: load_image, load_psf
  General type: load_table, load_table_model, load_user_model

- Multiple Datasets - data id

  Default data id =1
  load_data(2, “data2.dat”, ncols=3)

Help file:
load_data([id=1], filename, [options])
load_image([id=1], filename|IMAGECrate,[coord="logical"])

Examples:
load_data("src", "data.txt", ncols=3)

load_data("rprofile_mid.fits[cols RMID,SUR_BRI,SUR_BRI_ERR]")
load_data(“image.fits”)
load_image(“image.fits”, coord=“world”))

- Filtering the data
  load_data expressions
  notice/ignore commands in Sherpa

Examples:
notice(0.3,8)
notice2d("circle(275,275,50)")

Models in Sherpa

- Parameterized models: $f(x_i, p_k)$

  absorption - N_H

  photon index of a power law function - Γ

  blackbody temperature kT

- Library of models

```
sherpa> list_models()
['absorptionedge',
 'absorptiongaussian',
'atten',
'bbody',
 'bbodyfreq',
 'beta1d',
 'beta2d',
 'blackbody',
.........
```

- User Models can be added
- Model language to build compound model expressions

Building Models: Expressions

- Standard operations: + - * :
- Linking parameters: link()
- Convolution:
    - responses, arf & rmf files via standard I/O
    - PSF - an image file or a Sherpa model
    - load_conv() - a generic kernel from a file or defined by a Sherpa model

Building Models: Examples

- Building composite models:
  - models in the library: e.g. *powlaw1d, atten*
  - give a name for a model component in the expression:

```
set_source(1,'atten.abs1*atten.abs2*powlaw1d.p1')
set_source(2,'abs1*abs2*powlaw1d.p2')
```

- Building a model expression with convolved and unconvolved components:

```
set_full_model(1,'psf(gauss2d.g2)+const2d.c1')
```

Building Models: Examples

- Source and Background models:

```
set_source(2,'xsphabs.abs1*(powlaw1d.p1+gauss1d.g1)')
set_bkg_model(2,'const1d.mybkg')
```

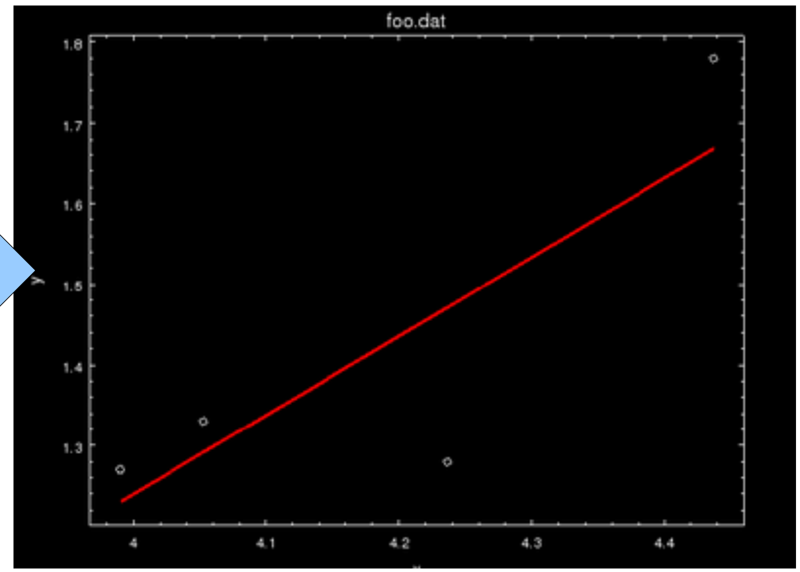
User Models: Python Function

- Adding a user model defined as 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
```



User Models: Tables

- `load_table_model()`
- The file may be 1D data from a FITS table, ASCII table data, or 2D data from a FITS image file.
    - modelname - the name for the table model
    - filename - the name of the file which contains the data
    - ncols (table input) - number of columns to read;
    - colkeys (table input) - list of column names;
    - dstype (table input) - dataset type: *Data1D, Data1DInt, Data2D, Data2DInt;*
    - coord (image input) - the coordinate system: *logical, image, physical, world, or wcs;*
    - method - interpolation method in sherpa.utils:

      linear_interp, nearest_interp, neville, neville2d;

```
sherpa> load_table_model("emap", "expmap.fits")
```

User Models: XSPEC Table Model

```
load_xstable_model("pul", "coplrefl.fits")
set_source(xsphabs.galabs * pul)
pul.xi = 1.5
pul.e_cut = 25
```

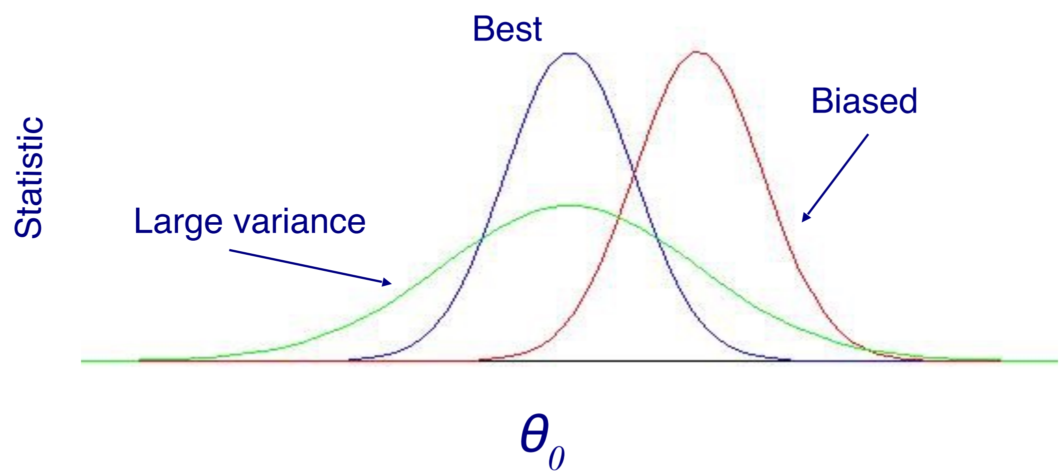
XSPEC table model coplrefl.fits is input as pul and used in the model expression.

```
show_source()
Model: 1
(xsphabs.galabs * xstablemodel.pul)
   Param        Type          Value          Min          Max      Units
   -----        ----          -----          ---          ---      -----
   galabs.nH    thawed            1            0       100000 10^22 atoms / cm^2
   pul.xi       thawed          1.5        1.477        3.977
   pul.gamma    thawed            1          0.5          1.5
   pul.e_cut    thawed           25            5           30
   pul.e_fold   thawed           15            5           30
   pul.redshift frozen            0            0            5
   pul.norm     thawed            1            0        1e+24
```

Fit Statistics in Sherpa

Fit statistics - math operation on data and model arrays

```
In [19]: list_stats()
Out[19]:
['cash',
 'chi2',
 'chi2constvar',
 'chi2datavar',
 'chi2gehrels',
 'chi2modvar',
 'chi2xspecvar',
 'cstat',
 'leastsq',
 'userstat',
 'wstat']
In [20]: set_stat('cash')
```

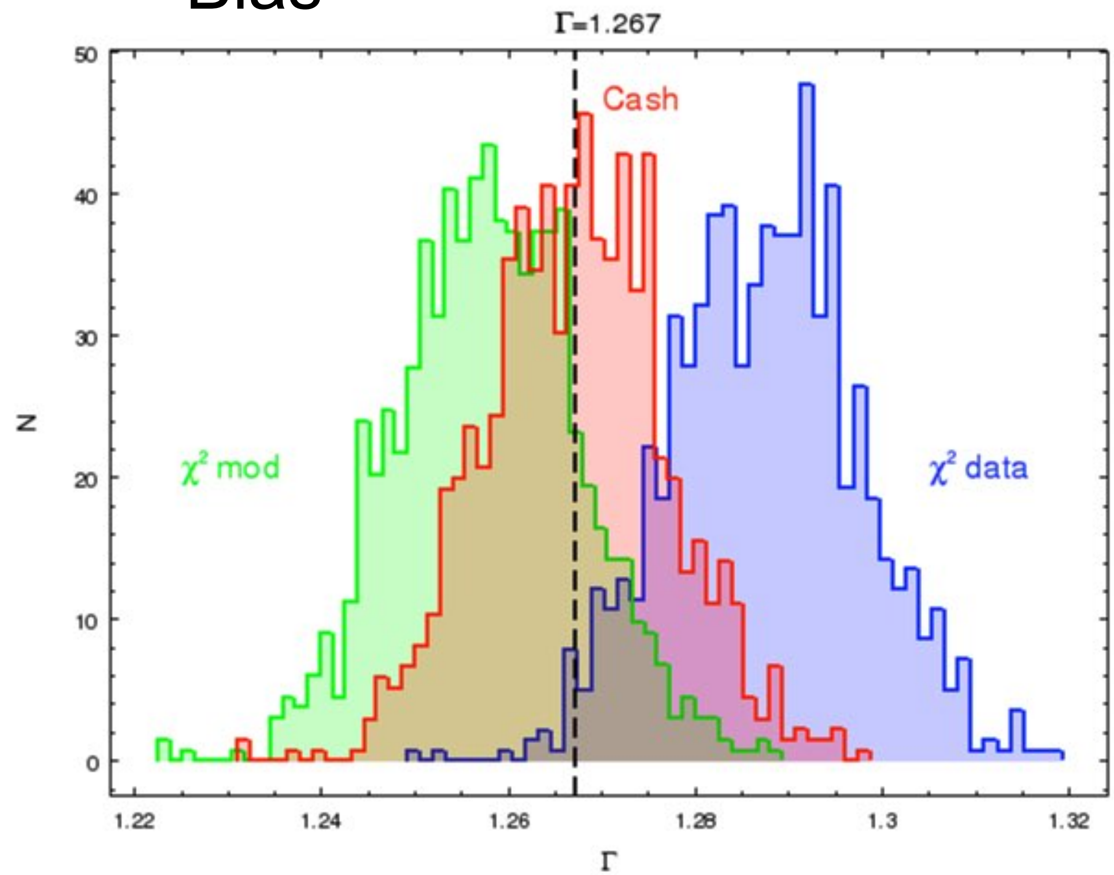


chi2 statistics as defined by different weights
and Poisson likelihood - cash/cstat/wstat

Fit Statistics in Sherpa

```
In [19]: list_stats()
Out[19]:
['cash',
 'chi2',
 'chi2constvar',
 'chi2datavar',
 'chi2gehrels',
 'chi2modvar',
 'chi2xspecvar',
 'cstat',
 'leastsq',
 'userstat',
 'wstat']
In [20]: set_stat('cash')
```

Bias



"Handbook of X-ray Astronomy "
(2011), Arnaud, Smith, Siemiginowska

Fitting: Search in the Parameter Space

sherpa-28> fit()

```
Dataset              = 1
Method               = levmar
Statistic            = chi2datavar
Initial fit statistic = 644.136
Final fit statistic   = 632.106 at function evaluation 13
Data points          = 460
Degrees of freedom     = 457
Probability [Q-value] = 9.71144e-08
Reduced statistic      = 1.38316
Change in statistic    = 12.0305
   zabs1.nh       0.0960949
   p1.gamma       1.29086
   p1.ampl        0.000707365
```

sherpa-29> print get_fit_results()

```
datasets   = (1,)
methodname = levmar
statname   = chi2datavar
succeeded  = True
parnames   = ('zabs1.nh', 'p1.gamma', 'p1.ampl')
parvals    = (0.0960948525609, 1.29085977295, 0.000707365006941)
covarerr   = None
statval    = 632.10587995
istatval   = 644.136341045
dstatval   = 12.0304610958
numpoints  = 460
dof        = 457
qval       = 9.71144259004e-08
rstat      = 1.38316385109
message    = both actual and predicted relative reductions in the sum of
squares are at most
ftol=1.19209e-07
nfev       = 13
```

Fitting: Sherpa Optimization Methods

- Optimization - a minimization of a function:

  "*A general function $f(x,p)$ may have* ***many isolated local minima****, non-isolated minimum hypersurfaces, or even more complicated topologies. No finite minimization routine can guarantee to locate the unique, global, minimum of $f(x,p)$ without being fed intimate knowledge about the function by the user.*"

- Therefore:

1. Never accept the result using a single optimization run; always test the minimum using a different method.
2. Check that the result of the minimization does not have parameter values at the edges of the parameter space. If this happens, then the fit must be disregarded since the minimum lies outside the space that has been searched, or the minimization missed the minimum.
3. Get a feel for the range of values of the fit statistic, and the stability of the solution, by starting the minimization from several different parameter values.
4. Always check that the minimum "looks right" using a plotting tool.

Fitting: Optimization Methods in Sherpa

- "Single - shot" routines: Simplex and Levenberg-Marquardt

  start from a set of parameters, and then improve in a continuous fashion:

  - Very Quick
  - Depend critically on the initial parameter values
  - Investigate a local behaviour of the statistics near the initial parameters, and then make another guess at the best direction and distance to move to find a better minimum.
  - Continue until all directions result in increase of the statistics or a number of steps has been reached

- "Scatter-shot" routines: moncar (differential evolution)

  search over the entire permitted parameter space for a better minima than near the starting initial set of parameters.

- Bayesian sampling methods: Markov-Chain Monte Carlo

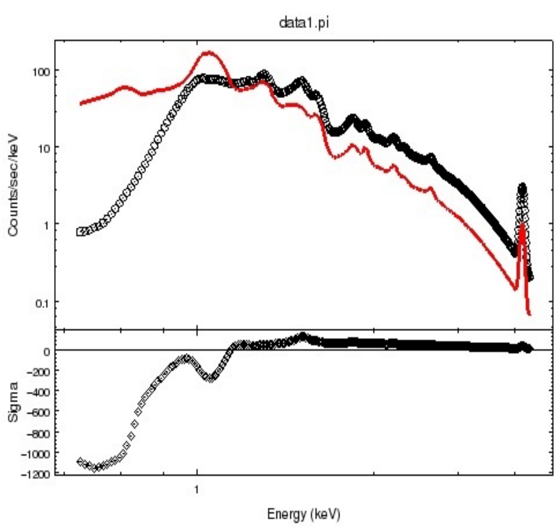
Optimization Methods: Comparison

Example: Spectral Fit with 3 methods

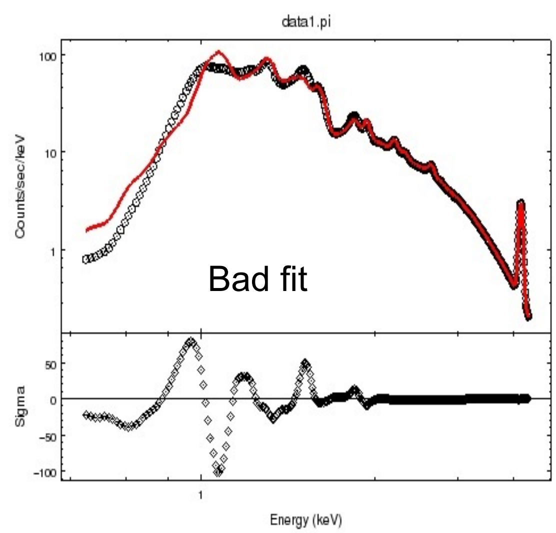
Data: high S/N simulated ACIS-S spectrum of the two temperature plasma
Model: photoelectric absorption plus two MEKAL components (correlated!)

Start fit from the same initial parameters
Figures and Table compares the efficiency and final results

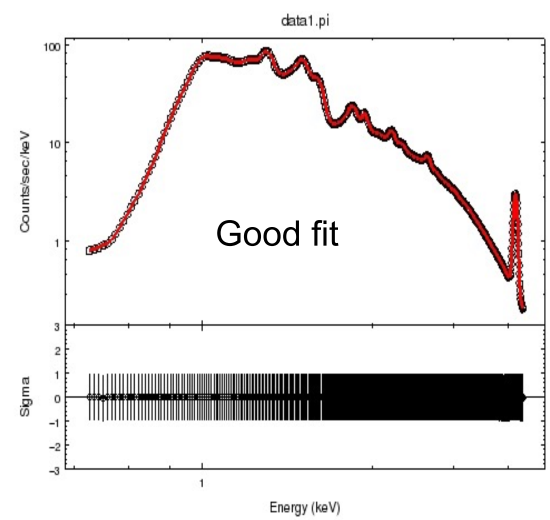
Method	Number of Iterations	Final Statistics
Levmar	31	1.55e5
Neldermead	1494	0.0542
Moncar	13045	0.0542



Data and Model with initial parameters



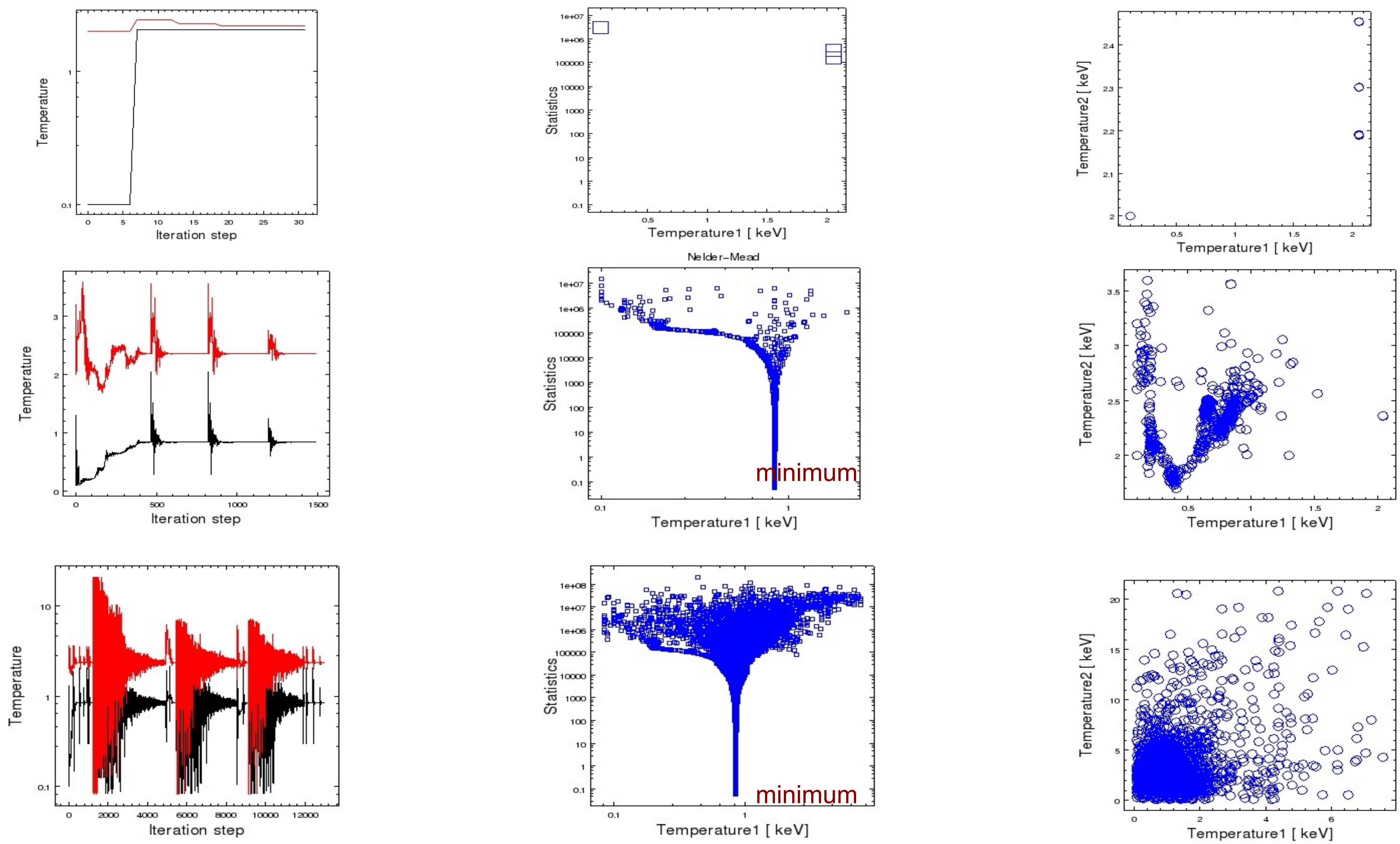
Levmar fit



Nelder-Mead and Moncar fit

Optimization Methods: Probing Parameter Space

	Temperature	Statistics vs. Temperature	2D slice of Parameter Space probed by each method
levmar			
simplex			
moncar			



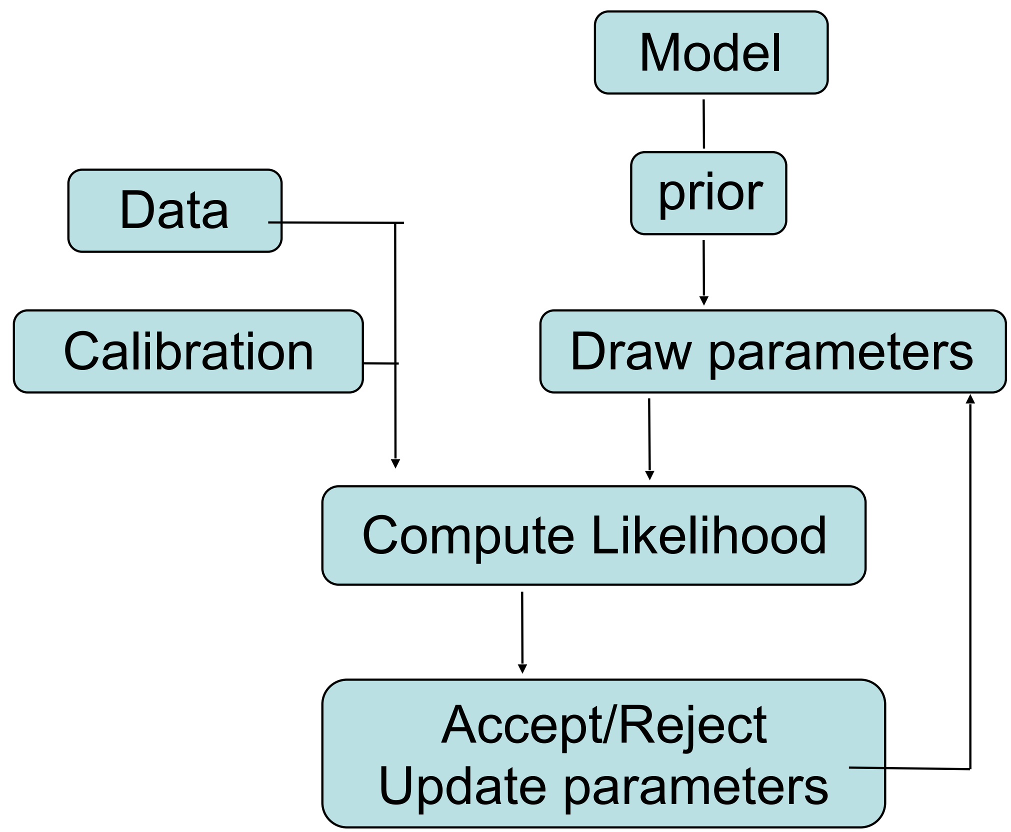
Sherpa, MCMC and Bayesian Analysis

MCMC samplers in Sherpa:

Metropolis and Metropolis-Hastings algorithms

Support for the Bayesian analysis with priors.

- Explores parameter space and summarizes the full posterior or profile posterior distributions.
- Computed parameter uncertainties can include systematic or calibration errors.
- Simulates replicate data from the posterior predictive distributions.



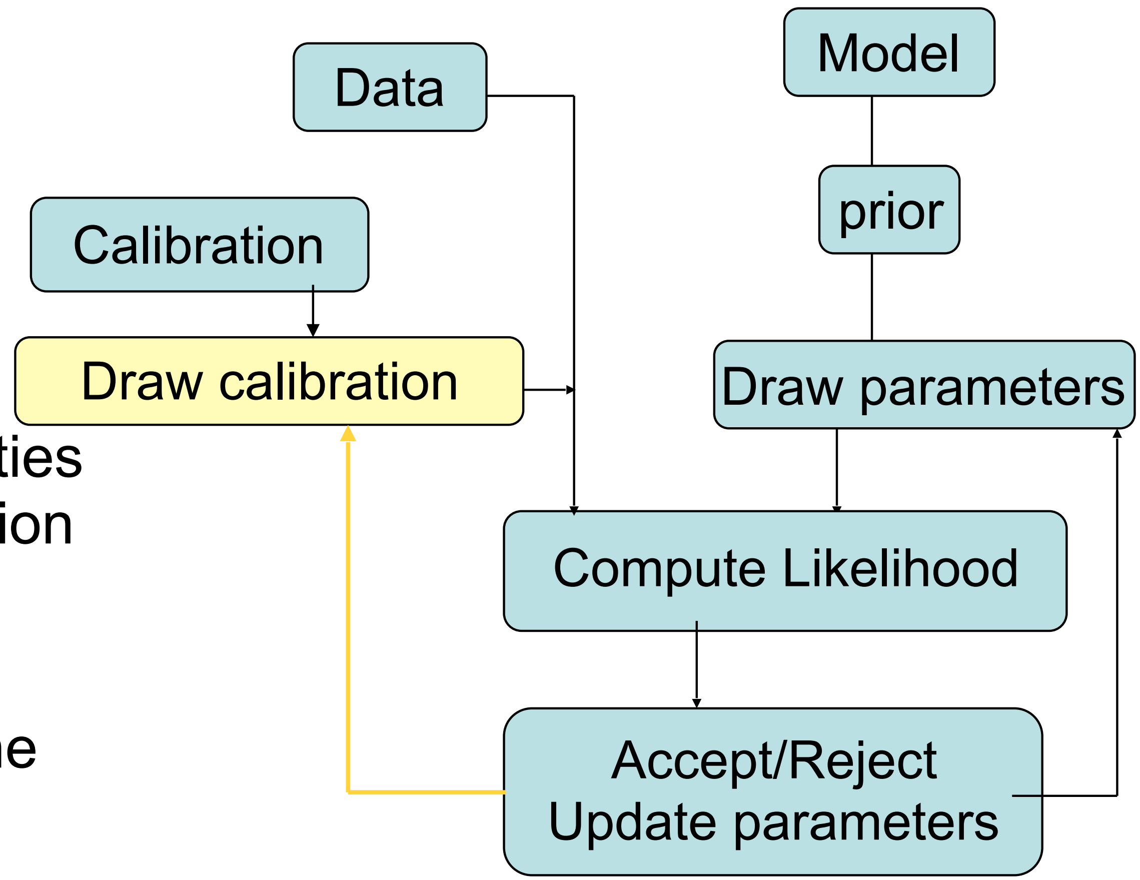
Sherpa, MCMC and Bayesian Analysis

MCMC samplers:

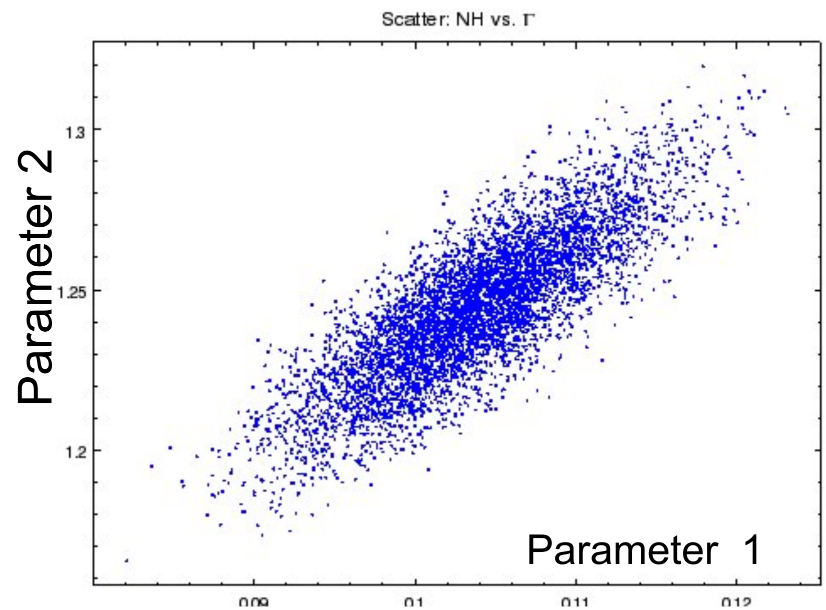
Metropolis and Metropolis-Hastings algorithms

Support for Bayesian analysis with priors.

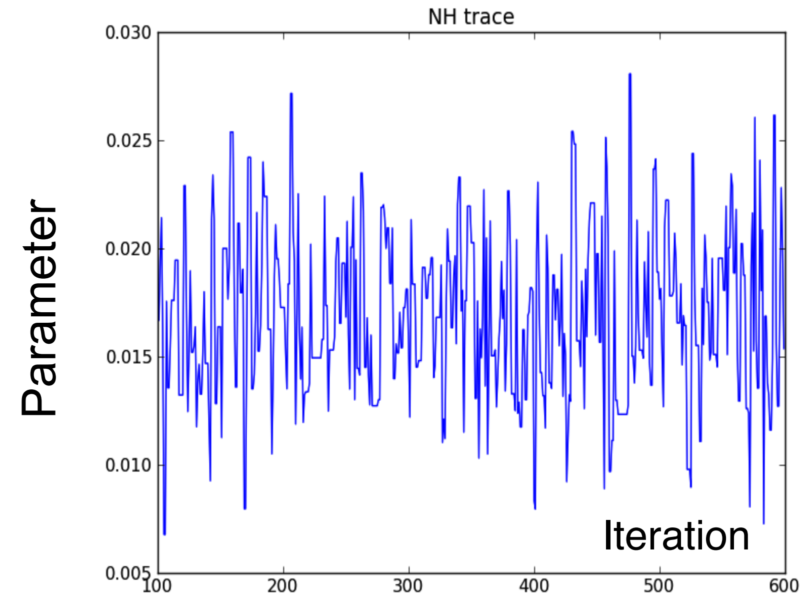
- Explores parameter space and summarizes the full posterior or profile posterior distributions.
- Computed parameter uncertainties can include systematic or calibration errors.
- Simulates replicate data from the posterior predictive distributions.

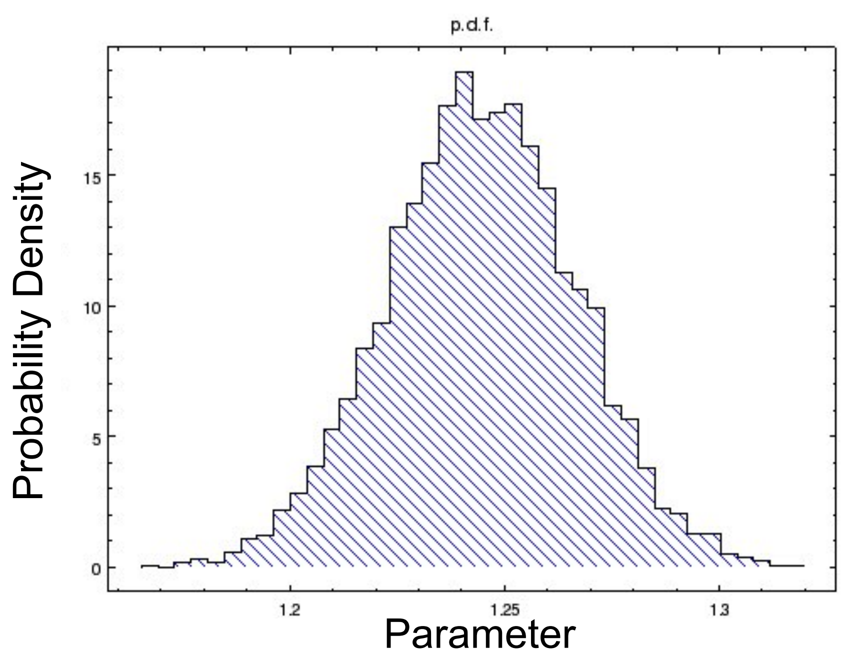


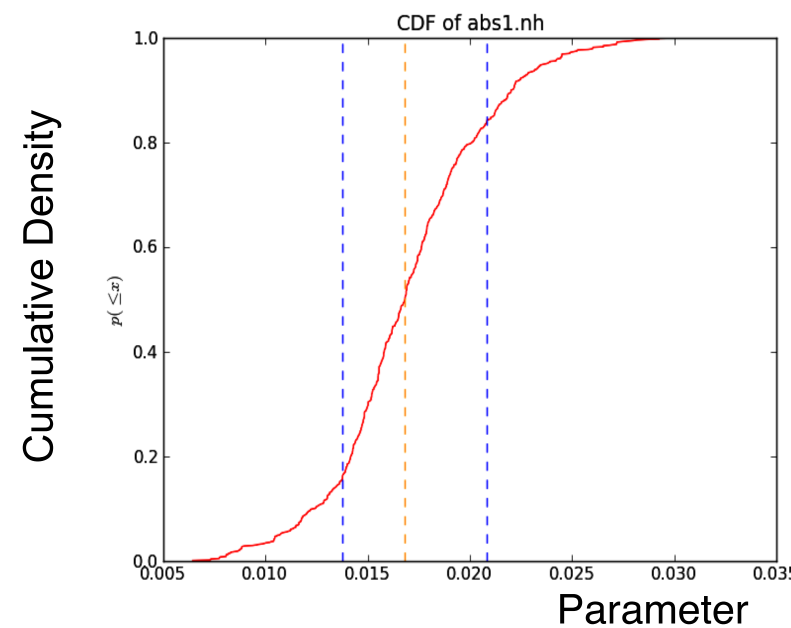
Visualization of the MCMC Results



Trace of a parameter during MCMC run







Final Analysis Steps

- How well are the model parameters constrained by the data?
- Is this a correct model?
- Is this the only model?
- Do we have definite results?
- What have we learned, discovered?
- How our source compares to the other sources?
- Do we need to obtain a new observation?

Confidence Limits

Essential issue = after the bets-fit parameters are found estimate the confidence limits for them. The region of confidence is given by (Avni 1976):

$$\chi^2_\alpha = \chi^2_{min} + \Delta(\nu,\alpha)$$

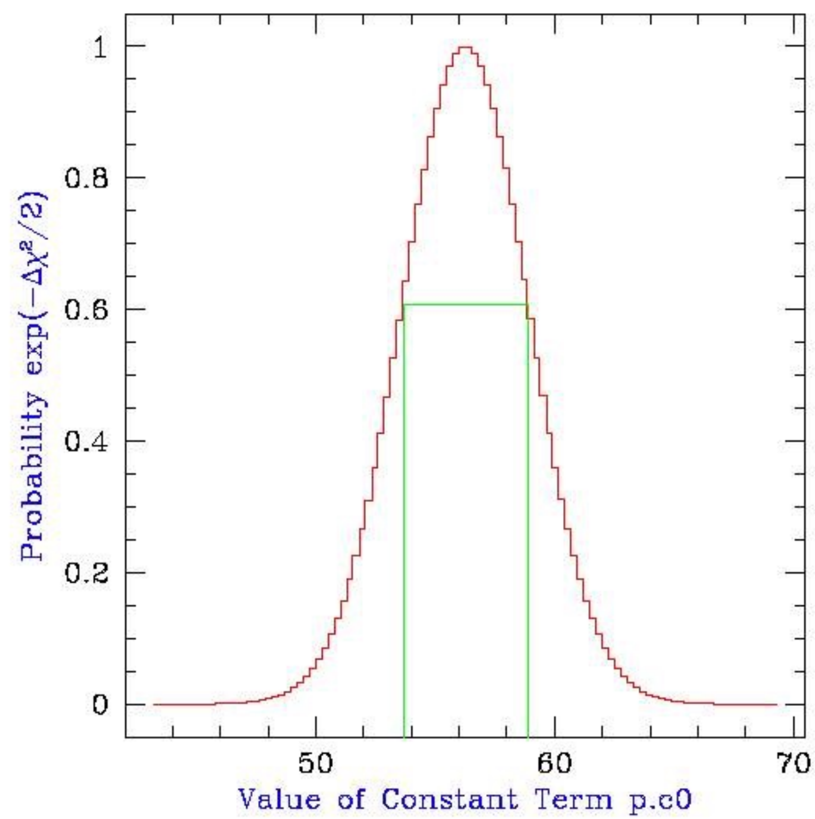
ν - degrees of freedom
α - level
χ^2_{min} - minimum

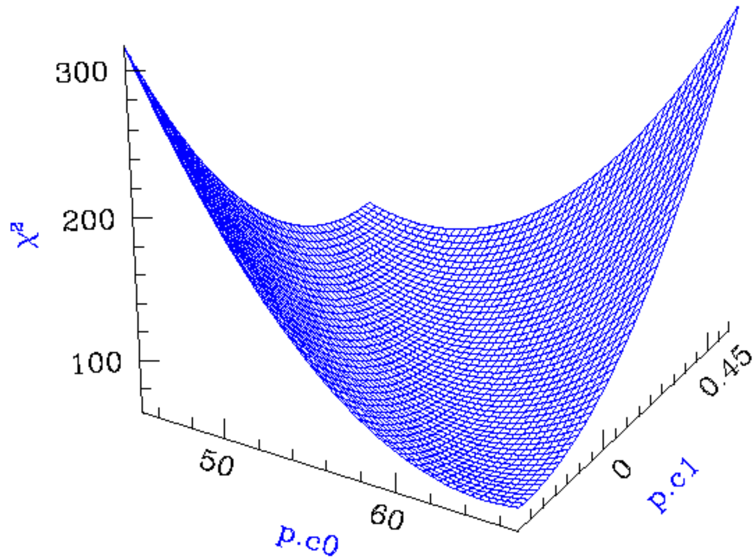
Δ depends only on the number of parameters involved not on goodness of fit

TABLE 1

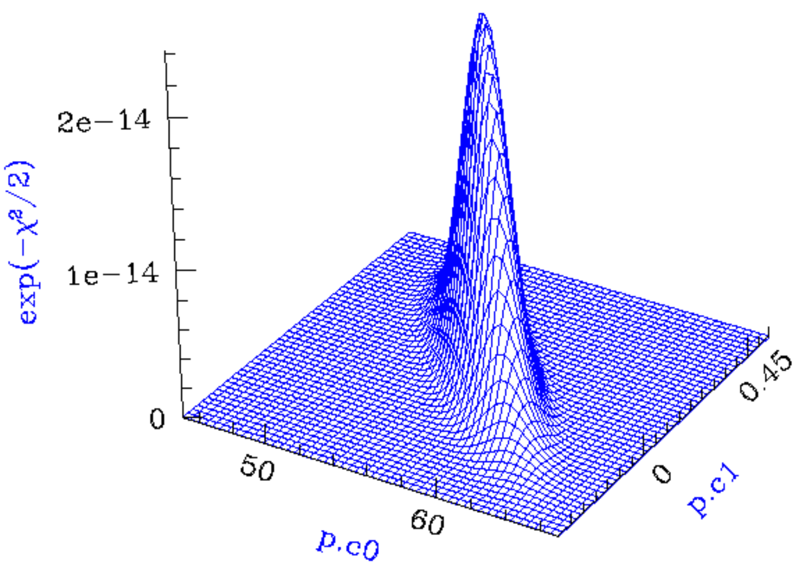
CONSTANTS FOR CALCULATING CONFIDENCE REGIONS

α (%)	q (No. of Interesting Parameters) 1	2	3
68.........	1.00	2.30	3.50
90.........	2.71	4.61	6.25
99.........	6.63	9.21	11.30





Calculating Confidence Limits
means
Exploring the Parameter Space - Statistical Surface



Example of a "well-behaved" statistical surface in parameter space, viewed as a multi-dimensional paraboloid (χ^2, *top*), and as a multi-dimensional Gaussian (exp(-χ^2 /2) $\approx \mathcal{L}$, *bottom*).

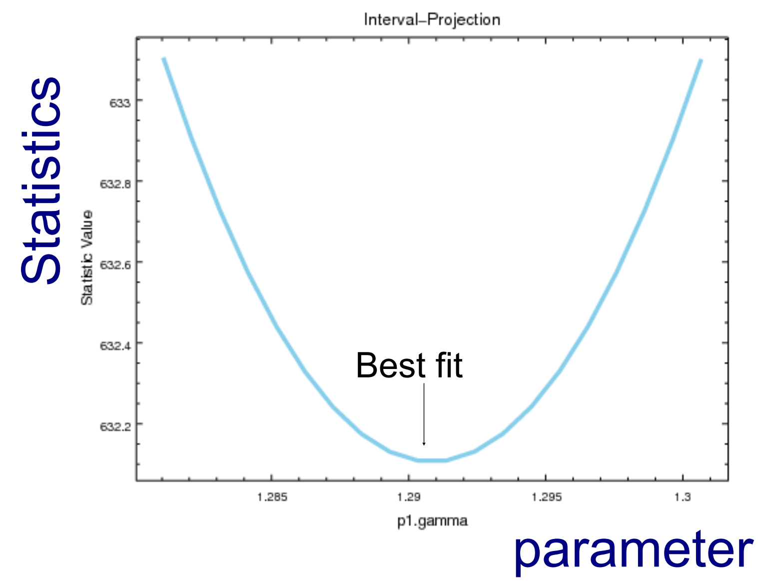
Confidence Intervals

sherpa-40> **covariance()**

```
Dataset              = 1
Confidence Method    = covariance
Fitting Method       = neldermead
Statistic            = chi2datavar
covariance 1-sigma (68.2689%) bounds:
   Param            Best-Fit  Lower Bound  Upper Bound
   -----            --------  -----------  -----------
   abs1.nH            1.1015  -0.00153623   0.00153623
   mek1.kT          0.841024  -0.00115618   0.00115618
   mek1.norm        0.699764  -0.00395776   0.00395776
   mek2.kT           2.35844  -0.00371253   0.00371253
   mek2.norm         1.03725  -0.00172503   0.00172503
```

sherpa-42> **conf()**

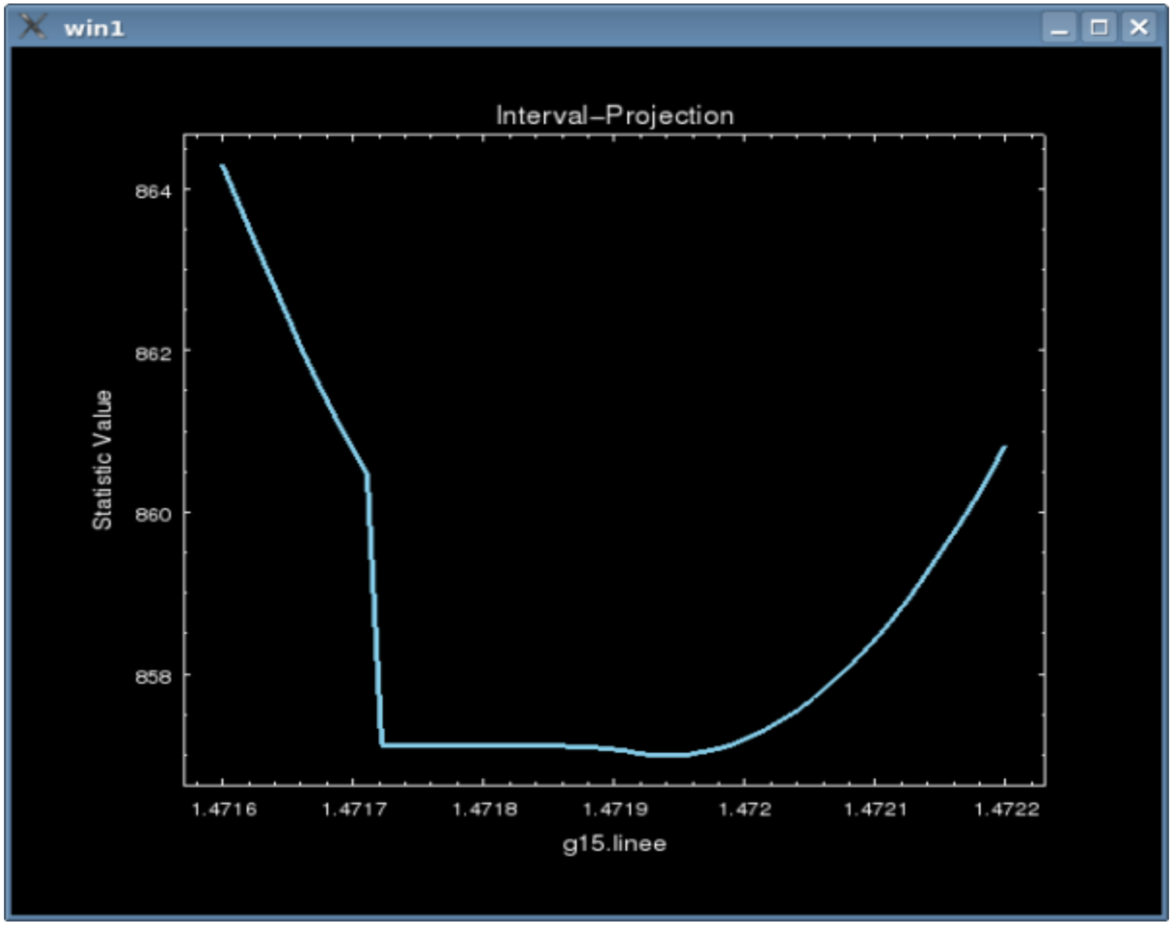
```
mek1.kT lower bound:    -0.00113811
mek1.kT upper bound:    0.0011439
mek2.kT lower bound:    -0.00365452
mek2.kT upper bound:    0.00364805
mek1.norm lower bound:  -0.00377224
mek2.norm lower bound:  -0.00164417
mek2.norm upper bound:  0.00164816
abs1.nH lower bound:    -0.00147622
mek1.norm upper bound:  0.00376011
abs1.nH upper bound:    0.00147268
Dataset              = 1
Confidence Method    = confidence
Fitting Method       = neldermead
Statistic            = chi2datavar
confidence 1-sigma (68.2689%) bounds:
   Param            Best-Fit  Lower Bound  Upper Bound
   -----            --------  -----------  -----------
   abs1.nH            1.1015  -0.00147622   0.00147268
   mek1.kT          0.841024  -0.00113811    0.0011439
   mek1.norm        0.699764  -0.00377224   0.00376011
   mek2.kT           2.35844  -0.00365452   0.00364805
   mek2.norm         1.03725  -0.00164417   0.00164816
```



sherpa-42> **print get_conf_results()**

```
----------> print(get_conf_results())
datasets   = (1,)
methodname = confidence
fitname    = neldermead
statname   = chi2datavar
sigma      = 1
percent    = 68.2689492137
parnames   = ('abs1.nH', 'mek1.kT', 'mek1.norm', 'mek2.kT', 'mek2.norm')
parvals    = (1.1015003421601872, 0.84102381214069499, 0.69976355976410642,
2.3584395600380756, 1.0372453037692799)
parmins    = (-0.0014762187156509565, -0.0011381111192153346,
-0.0037722356859711814, -0.0036545192286010497, -0.0016441656050858455)
parmaxes   = (0.0014726797455479889, 0.0011439029752089436,
0.0037601110158367312, 0.0036480458191339916, 0.0016481622297106488)
nfits      = 103
```

Not well-behaved Surface

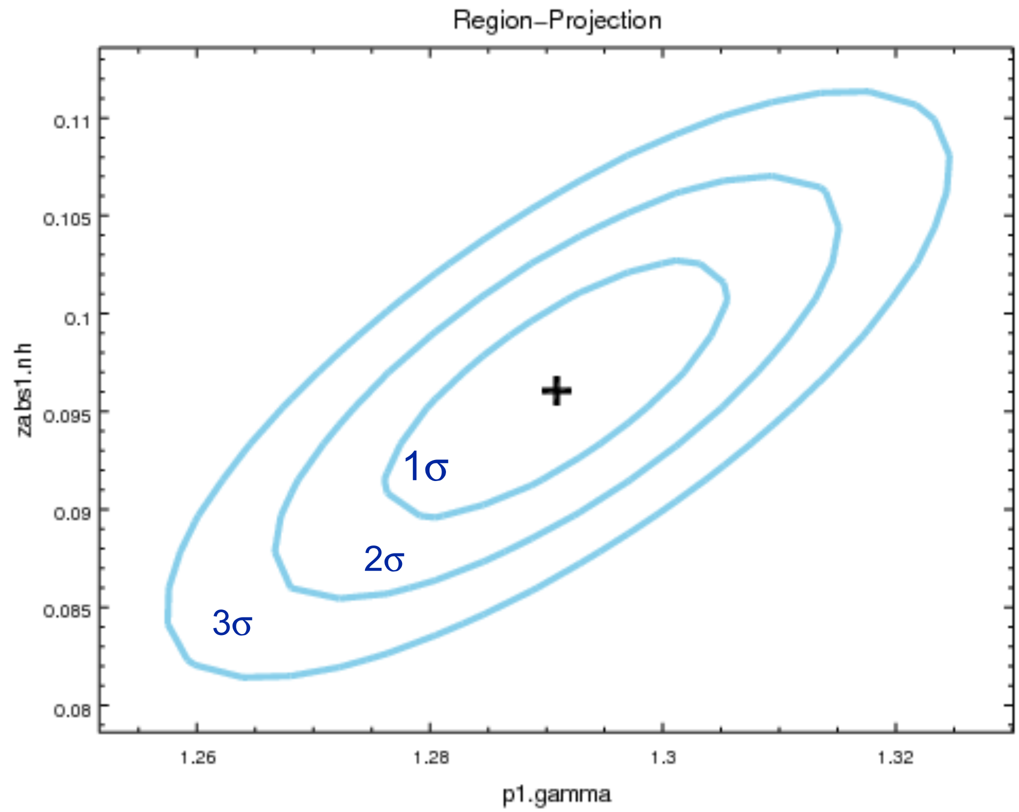


Non-Gaussian Shape

Confidence Regions

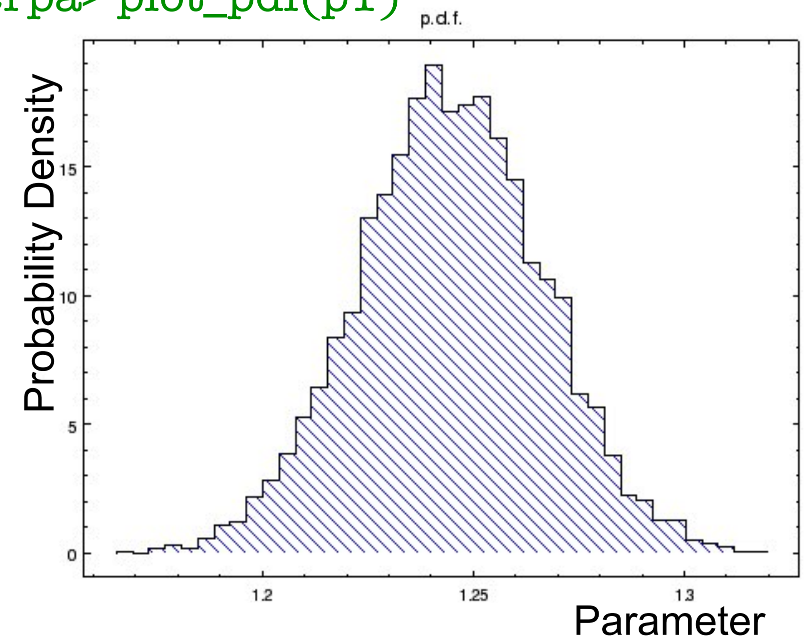
sherpa-61> **reg_proj(p1.gamma,zabs1.nh,nloop=[20,20])**
sherpa-62> **print get_reg_proj()**

```
min     = [ 1.2516146   0.07861824]
max     = [ 1.33010494  0.11357147]
nloop   = [20, 20]
fac     = 4
delv    = None
log     = [False False]
sigma   = (1, 2, 3)
parval0 = 1.29085977295
parval1 = 0.0960948525609
levels  = [ 634.40162888  638.28595426  643.93503803]
```

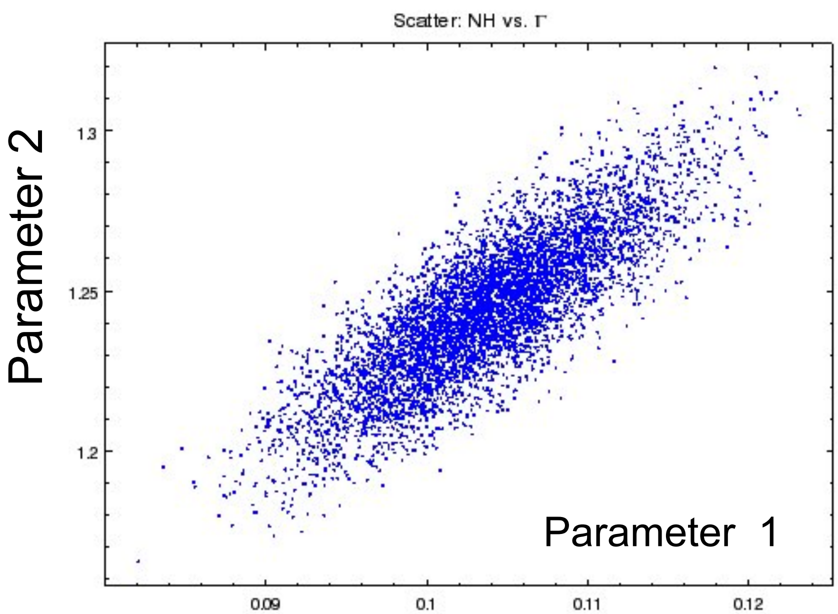


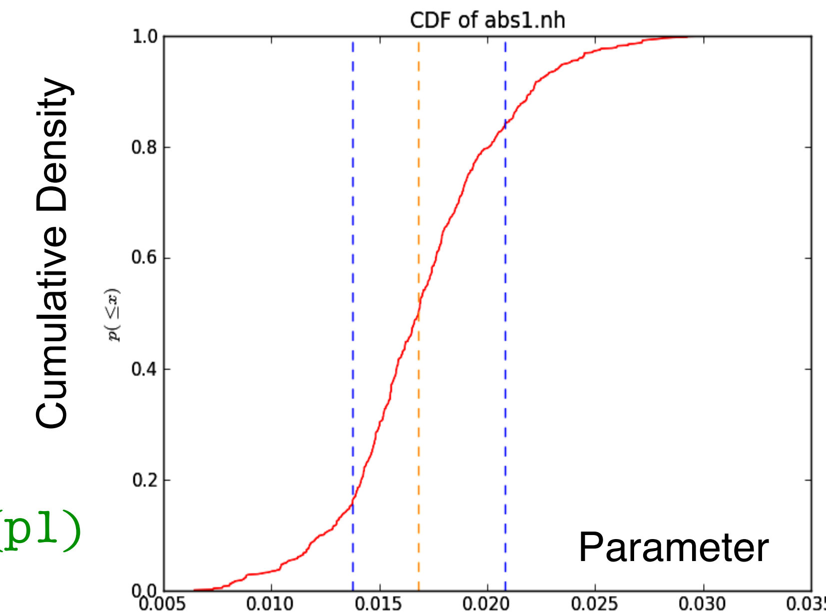
MCMC Results: Probability Distributions

sherpa> plot_pdf(p1)



sherpa> plot_scatter(p1,p2)





sherpa> plot_cdf(p1)

Distributions of Flux and Parameters

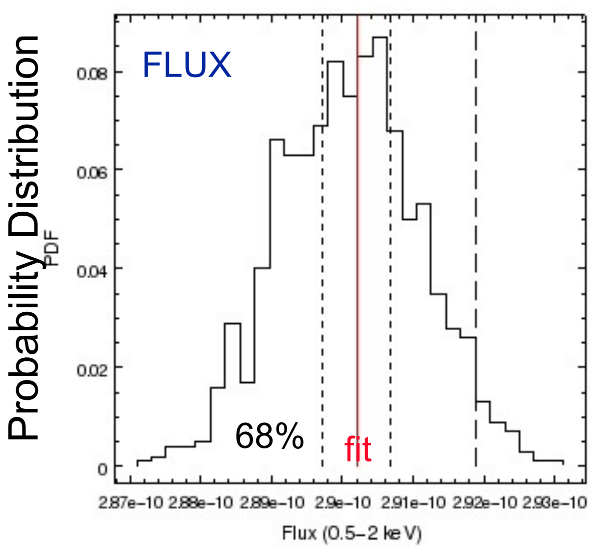
Functions: sample_energy_flux, sample_flux

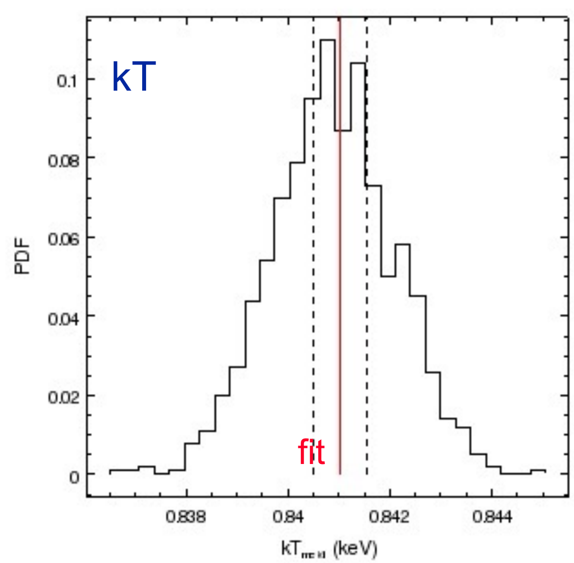
Monte Carlo Simulations of parameters assuming Gaussian distributions for all the parameters
Characterized by the covariance matrix, includes correlations between parameters.

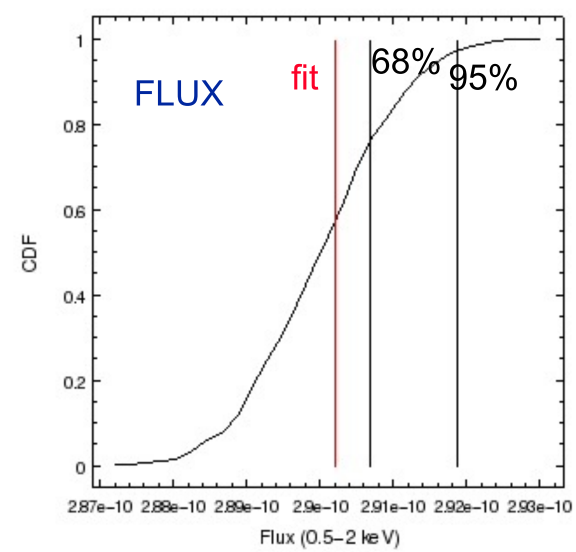
```
sherpa-19> flux100=sample_energy_flux(0.5,2.,num=100)
sherpa-20> print flux100
---------> print(flux100)
[[  2.88873592e-10   1.10331438e+00   8.40356670e-01   6.97503733e-01
    2.35411369e+00   1.03580042e+00]
 [  2.90279483e-10   1.10243140e+00   8.41174148e-01   7.01009661e-01
 sherpa-26> plot_energy_flux(0.5,2,num=1000)
```

* Characterize distributions: plot PDF and CDF and obtain Quatiles of 68% and 95%

```
sherpa-30> fluxes=numpy.sort(flux1000[:,0])
sherpa-31> a95=fluxes(0.95*len(flux1000[:,0])-1)
sherpa-32> a68=fluxes(0.68*len(flux1000[:,0])-1)
```







Sherpa - Summary

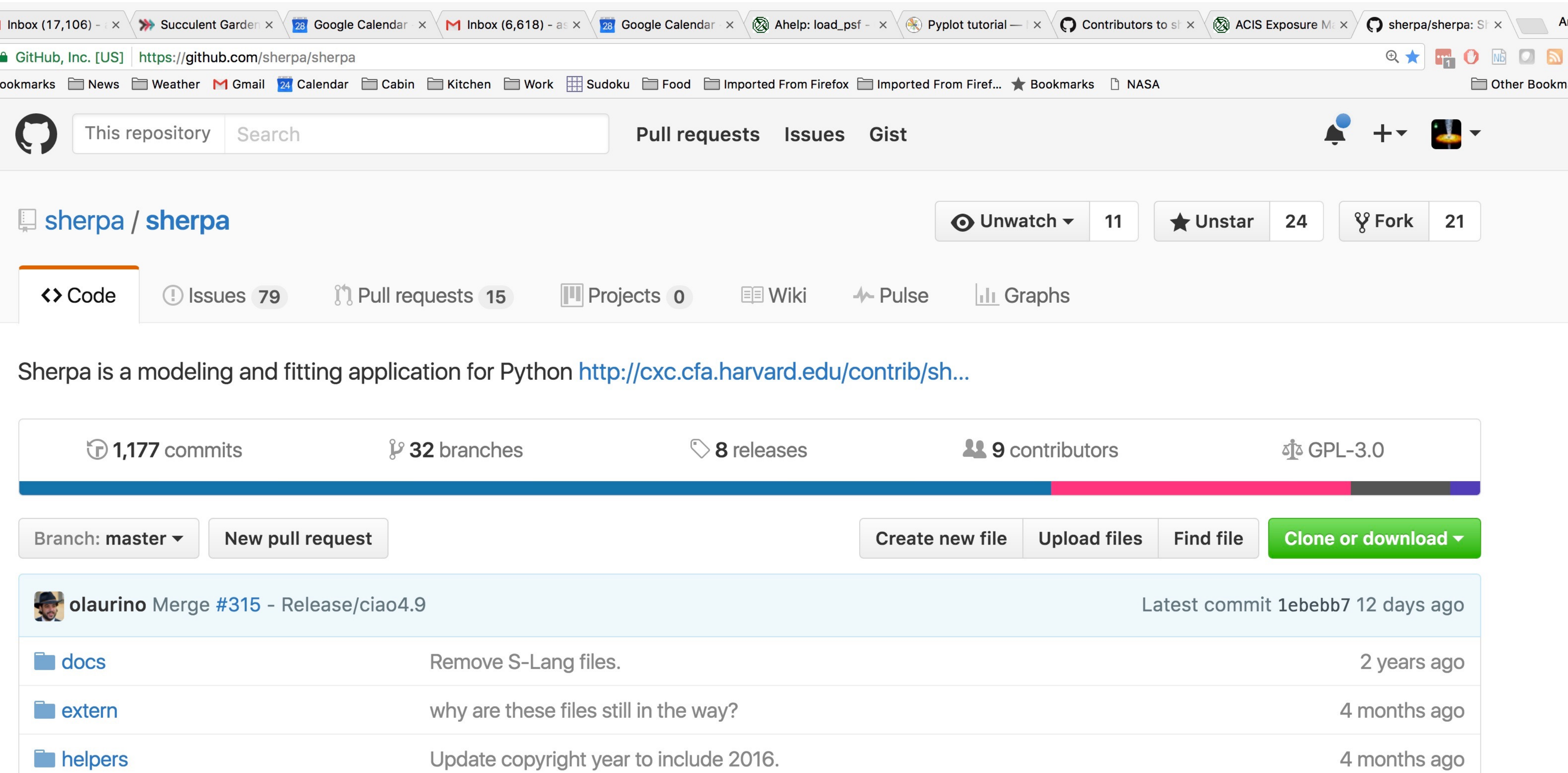
- Modeling and fitting application for Python.
- User Interface and high level functions written in Python.
- Modeling 1D/2D (N-D) data: arrays, spectra, images.
- Powerful language for building complex expressions.
- Provides a variety of statistics and optimization methods (including Bayesian analysis) .
- Support for wcs, responses, psf, convolution.
- Extensible to include user models, statistics and optimization methods.
- Included in several software packages.
- Source code on GitHub https://github.com/sherpa/sherpa
- Open development with continuous integration via Travis

Core Team:

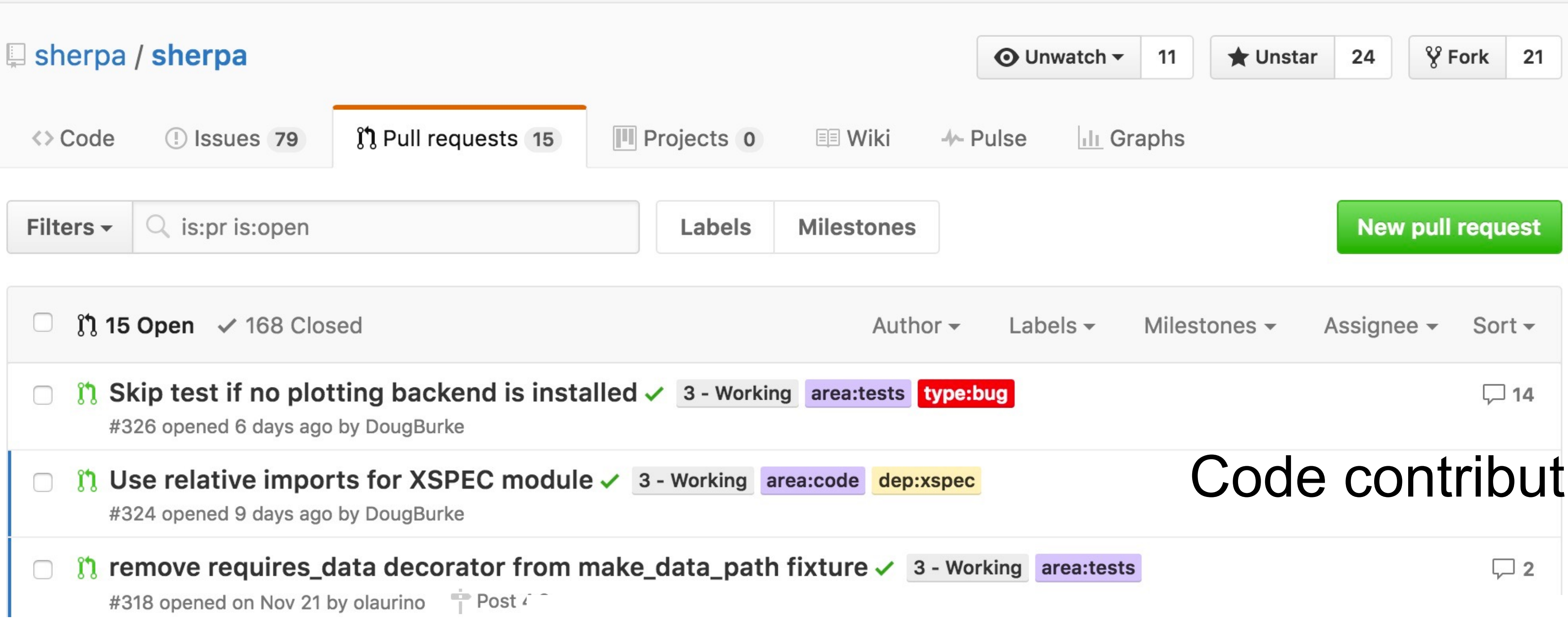
Omar Laurino, Doug Burke, Warren McLaughlin, Dan Nguyen, Aneta Siemiginowska

Code contributions:

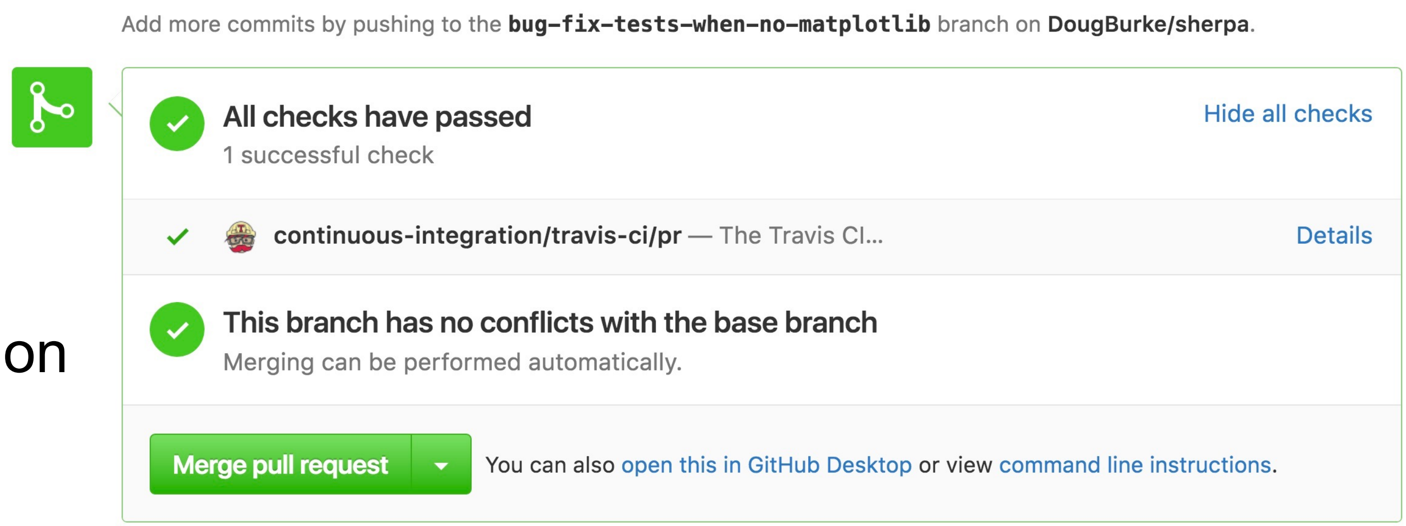
Tom Aldcroft, Jamie Budynkiewicz, Christoph Deil, Brigitta Sipocz



Open Development



Code contribution



Travis
- continuous integration

Using Sherpa in Astronomy Software

- IRIS - GUI for data exploration and SED fitting
  http://www.usvao.org/index.html%3Fpage_id=357.html
- BAX - Bayesian X-ray Analysis
  https://github.com/JohannesBuchner/BXA
- XMM-Newton Source Catalog:
  http://xmm-catalog.irap.omp.eu/docs/spectral-fitting
  - web interface to spectral fitting of the sources in 3XMM-DR6 catalog
- Astropy[a] Affiliated packages: http://www.astropy.org/affiliated/index.html
  - GammaPy https://gammapy.readthedocs.io/en/latest/
  - Naima https://naima.readthedocs.io/en/latest
- Saba - Sherpa-Astropy Bridge https://saba.readthedocs.io/en/latest/
  - Google funded a summer student (through GSOC program) to develop the code and documentation.
  - pending application for Astropy affiliated package.

a) From astropy.org web page:
Astropy is a community-driven package intended to contain much of the core functionality and some common tools needed for performing astronomy and astrophysics with Python.

Summary

- Sherpa is a Python package.
- It provides models, fit statistics and optimization methods for variety of problems in astronomy.
- It is flexible and extensible as it accepts new models, statistics or optimization.
- Sherpa can also be included in a modeling software in Python.

Learn more on Sherpa Web Pages

http://cxc.harvard.edu/sherpa

Freeman, P., Doe, S., & Siemiginowska, A. 2001, SPIE 4477, 76

Doe, S., et al. 2007, Astronomical Data Analysis Software and Systems XVI, 376, 543

Refsdal et al. 2009 - Sherpa: 1D/2D modeling and fitting in Python in Proceedings of the 8th Python in Science conference (SciPy 2009), G Varoquaux, S van der Walt, J Millman (Eds.), pp. 51-57

There are also Sherpa Jupyter Notebooks available on Sherpa GitHub page:

https://github.com/sherpa/sherpa/wiki

Example of Image Fitting:

http://nbviewer.jupyter.org/github/anetasie/SherpaNotebooks/blob/master/ImageFitting.ipynb

SABA: Sherpa - Astropy Bridge

- `astropy.modeling`
  - uses `scipy.optimize`, weighted least square, does not calculate uncertainties
- **SABA** https://saba.readthedocs.io/en/latest/
  - bridge between the model definition language in `astropy.modeling` and the powerful fitting capabilities of Sherpa.
- **Sherpa**
  - has a selection of robust optimization algorithms coupled with configurable fit statistics.
  - can estimate parameter confidence intervals, with methods that allow for coupled non-gaussian errors.
  - has an MCMC sampler that can be used to explore the posterior probability distribution.