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# Comparison of observed and theoretical Fe L emission from CIE plasmas

M. Carpenter, P. Beiersdorfer, G. V. Brown, H. C. Chen, M. F. Gu, J. G. Jernigan

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## **Comparison of observed and theoretical Fe L emission from CIE plasmas**

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We analyze data from the Lawrence Livermore National Lab (LLNL) Electron Beam Ion Trap (EBIT) that simulates a CIE plasma by sweeping the electron beam to approximate a Maxwellian velocity distribution. These results are compared to spectra of confirmed astronomical CIE plasmas (e.g. outer regions of x-ray clusters) observed by XMM/RGS. We utilize the Photon Clean Method (PCM) to quantify these spectra (EBIT and XMM/RGS) in the form of ratios of Fe L lines in the emission complex near 1 keV. The variances of line fluxes are measured with bootstrap methods (Efron 1979). Both of these observations are further compared with theoretical predictions of Fe L line fluxes from APED and similar atomic databases.

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# Comparison of Observed and Theoretical Fe L Emission from CIE Plasmas

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UC Berkeley Space Sciences Laboratory

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## Collaborators

### Lawrence Livermore National Lab Electron Beam Ion Trap (EBIT) Team

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H. Chen

### UC Berkeley Space Sciences Laboratory

J. G. Jernigan

X-Ray Spectroscopy Workshop  
Cambridge, MA

Matthew Carpenter, UCB SSL 7/11/2007,

# Overview

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- ❖ Introduction to the Photon Clean Method (PCM)
- ❖ An Example : XMM/RGS spectrum of Ab Dor
- ❖ PCM algorithm internals
- ❖ Analysis Modes: Phase I and Phase II solutions
- ❖ Bootstrap Methods of error analysis
- ❖ Summary

# Photon Clean Method: Principles

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- Analysis uses individual photon *events*, not binned spectra
- Fitting models to data is achieved through weighted random trial-and-error with feedback
- Individual photons span parameter and model space, and are taken to be the parameters
- Iteration until quantitative convergence based on a Kolmogorov-Smirnov (KS) test
- Has analysis modes which allow divergence from strict adherence to model to estimate differences between model and observed data

# Photon Clean Method: Event-Mode Data and Model

Both data and model are in form of Event Lists (photon lists)  
 Monte-Carlo methods are used to generate simulated photons

Generation parameters for each photon are recorded  $\longrightarrow$  Each photon is treated as independent parameter

Single simulated photon:

| $\lambda_{spec}(\text{\AA})$ | $\lambda_{sim}(\text{\AA})$ | $\log(T_{MK})$ | $T_{keV}$ | Type   | Transition                                  |
|------------------------------|-----------------------------|----------------|-----------|--------|---|
| 18.990                       | 18.967                      | 6.796          | 0.538     | O VIII | $2p \ ^2P_{3/2} \rightarrow 1s \ ^2S_{1/2}$ |

# PCM analyzes Simulated Detected $\lambda_{sim}$ or $E_{sim}$

| Observed Data<br>(Event Form)<br>$\lambda_{observed}(\text{\AA})$ | Simulated<br>Data<br>$\lambda_{sim}(\text{\AA})$ |
|---|--|
| 15.020  | 18.990   |
| 14.961  | 12.290   |
| 7.622   | 10.761   |
| 17.711  | 12.807   |
| 21.549  | 17.930   |
| 16.062  | 12.238   |
| 14.376  | 13.470   |
| 13.298  | 11.510   |
| 12.833  | 28.279   |
| 17.801  | 13.105   |
| 21.217  | 17.037   |
| ⋮   | ⋮  |

← Data representation inside program

**Target:** AB Dor (K1 IV-V), a young active star and XMM/RGS calibration target

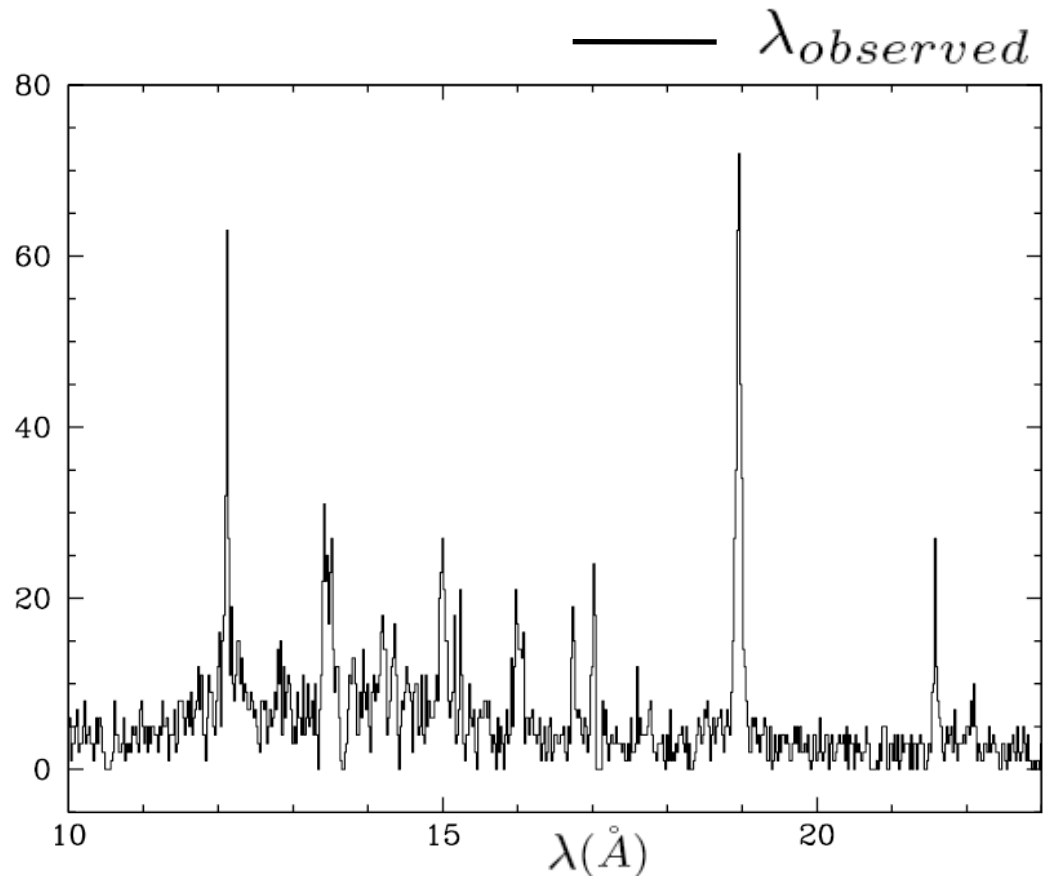


# PCM analyzes Simulated Detected $\lambda_{sim}$ or $E_{sim}$

**Target:** AB Dor (K1 IV-V), a young active star and XMM/RGS calibration target

**The Photon Clean Method algorithm analyzes and outputs models as event lists**  
**\*\*\* All histograms in this talk are for visualization only**

| $\lambda_{observed}(\text{\AA})$ | $\lambda_{sim}(\text{\AA})$ |
|----------------------------------|-----------------------------|
| 15.020                           | 18.990                      |
| 14.961                           | 12.290                      |
| 7.622                            | 10.761                      |
| 17.711                           | 12.807                      |
| 21.549                           | 17.930                      |
| 16.062                           | 12.238                      |
| 14.376                           | 13.470                      |
| 13.298                           | 11.510                      |
| 12.833                           | 28.279                      |
| 17.801                           | 13.105                      |
| 21.217                           | 17.037                      |
| ⋮                                | ⋮                           |



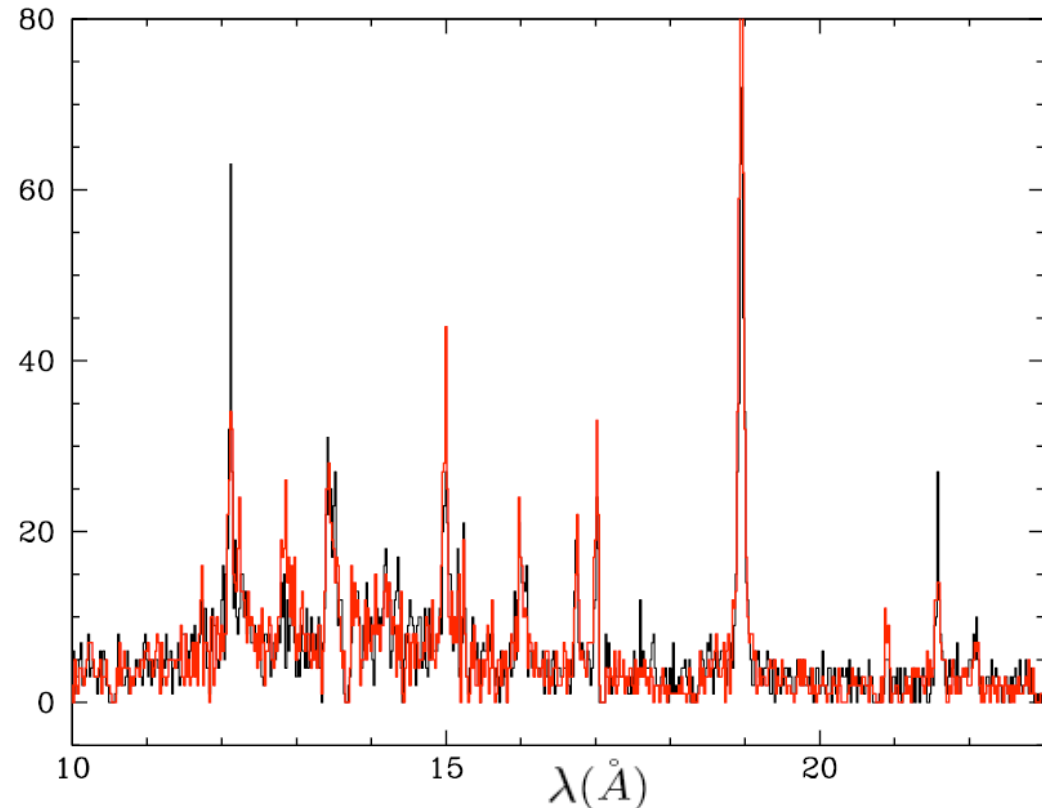
# PCM analyzes Simulated Detected $\lambda_{sim}$ or $E_{sim}$

**Target:** AB Dor (K1 IV-V), a young active star and XMM/RGS calibration target

**The Photon Clean Method algorithm analyzes and outputs models as event lists**  
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| 16.062                           | 12.238                      |
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| 12.833                           | 28.279                      |
| 17.801                           | 13.105                      |
| 21.217                           | 17.037                      |
| ⋮                                | ⋮                           |

—  $\lambda_{sim}$   
 —  $\lambda_{observed}$



# Spectral $\lambda$ : “Perfect” information

Each photon in a simulated observation has ideal (model) wavelength and the wavelength of detection

$\lambda_{spec}$  == “spectral wavelength”  
from plasma model

| Phot.# | $\lambda_{spec}(\text{\AA})$ | $\lambda_{sim}(\text{\AA})$ | $\log(T_{MK})$ | Type      |
|--------|------------------------------|-----------------------------|----------------|-----------|
| 1      | 18.990                       | 18.967                      | 6.796          | O VIII    |
| 2      | 12.903                       | 12.308                      | 6.839          | Continuum |
| 3      | 10.762                       | 10.849                      | 7.096          | Ni XXIII  |
| 4      | 12.806                       | 12.846                      | 7.129          | Fe XX     |
| 5      | 17.930                       | 18.037                      | 6.662          | Continuum |
| 6      | 12.238                       | 12.284                      | 7.030          | Fe XXI    |
| ⋮      | ⋮                            | ⋮                           | ⋮              | ⋮         |

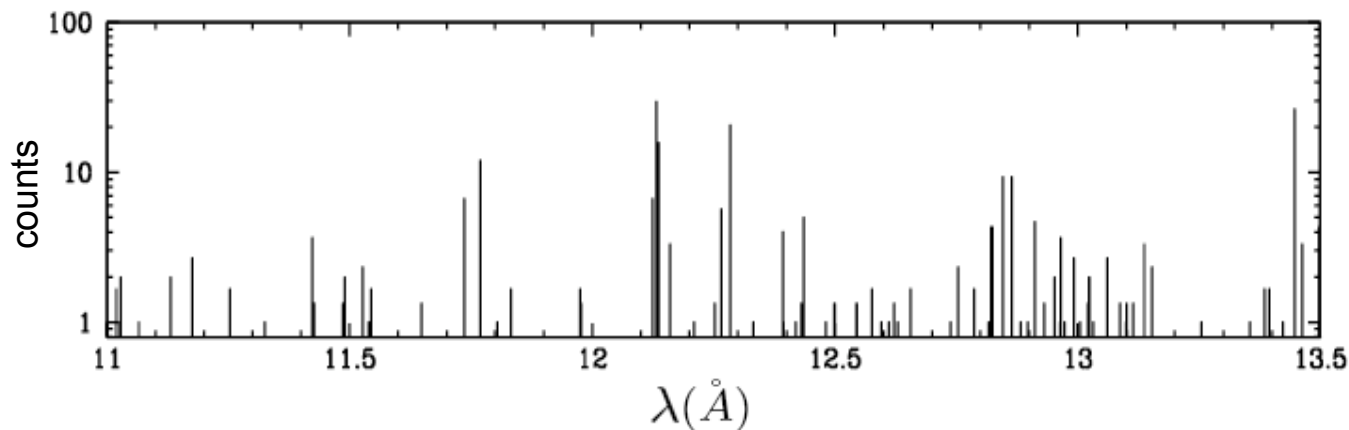
# Spectral $\lambda$ : “Perfect” information

Each photon in a simulated observation has ideal (model) wavelength and the wavelength of detection

$\lambda_{spec}$  == “spectral wavelength”  
from plasma model

A histogram of the simulated photons’ spectral wavelengths produces sharp lines

| Phot.# | $\lambda_{spec}(\text{\AA})$ | $\lambda_{sim}(\text{\AA})$ | $\log(T_{MK})$ | Type      |
|--------|------------------------------|-----------------------------|----------------|-----------|
| 1      | 18.990                       | 18.967                      | 6.796          | O VIII    |
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| ⋮      | ⋮                            | ⋮                           | ⋮              | ⋮         |



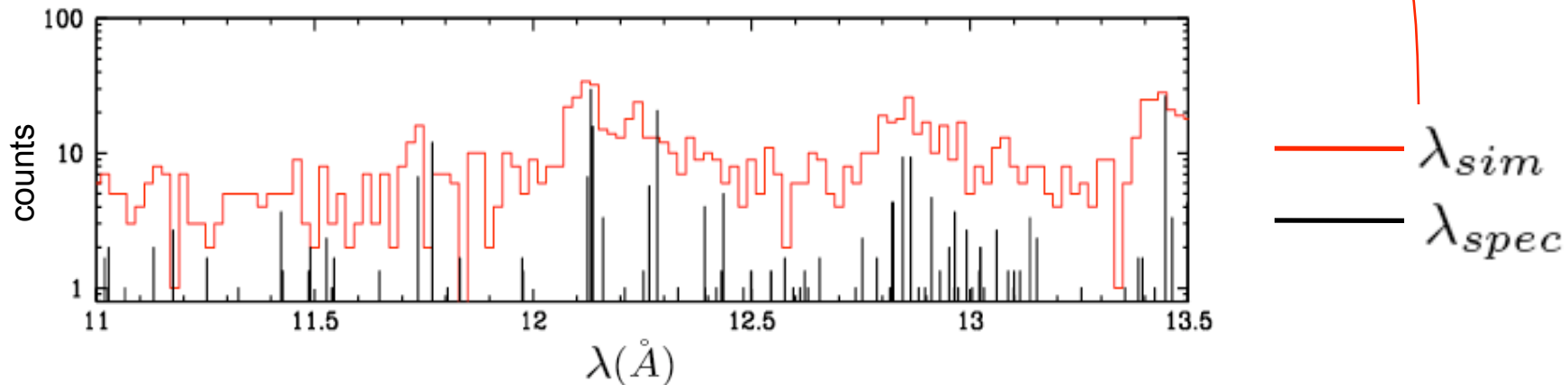
$\lambda_{spec}$

# Adding detector response

Photons are stochastically assigned a “detected wavelength”

$\lambda_{sim}$  == “simulated wavelength,” includes redshift, detector and thermal broadening

| Phot.# | $\lambda_{spec}(\text{\AA})$ | $\lambda_{sim}(\text{\AA})$ | $\log(T_{MK})$ | Type      |
|--------|------------------------------|-----------------------------|----------------|-----------|
| 1      | 18.990                       | 18.967                      | 6.796          | O VIII    |
| 2      | 12.903                       | 12.308                      | 6.839          | Continuum |
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| ⋮      | ⋮                            | ⋮                           | ⋮              | ⋮         |



# Distribution of Model Parameters

Each photon has individual parameter values which may be taken as elements of the parameter distribution

| Phot.# | $\lambda_{spec}(\text{\AA})$ | $\lambda_{sim}(\text{\AA})$ | log(T) | Type      |
|--------|------------------------------|-----------------------------|--------|-----------|
| 1      | 18.990                       | 18.967                      | 6.796  | O VIII    |
| 2      | 12.903                       | 12.308                      | 6.839  | Continuum |
| 3      | 10.762                       | 10.849                      | 7.096  | Ni XXIII  |
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| 6      | 12.238                       | 12.284                      | 7.030  | Fe XXI    |
| ⋮      | ⋮                            | ⋮                           | ⋮      | ⋮         |

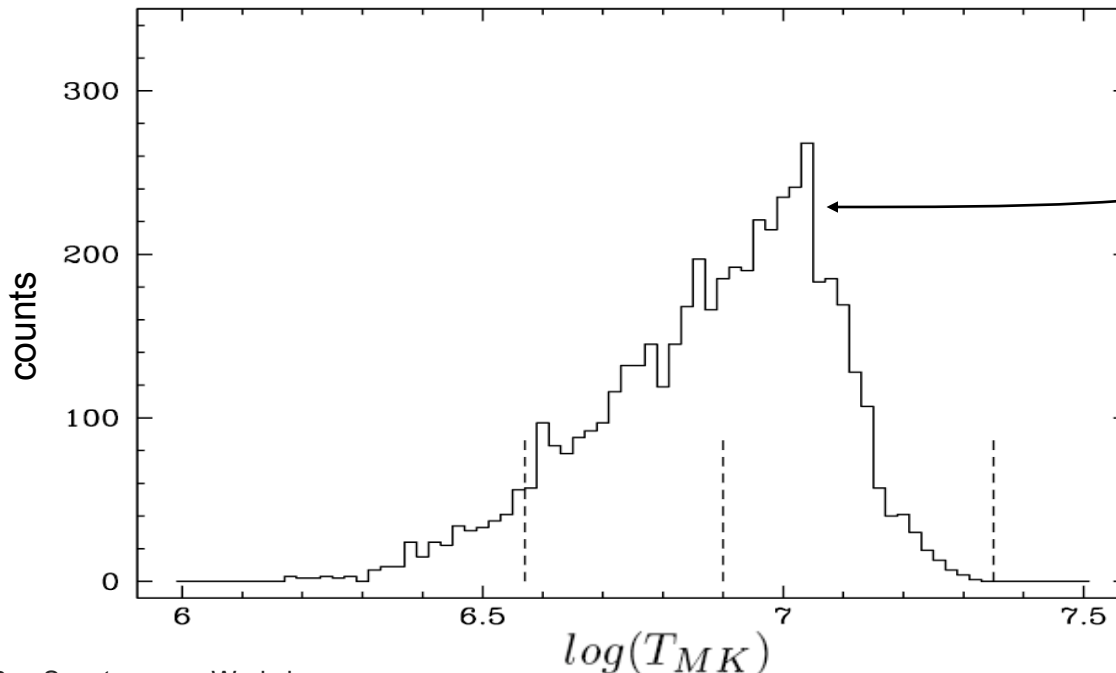
# Distribution of Model Parameters

Each photon has individual parameter values which may be taken as elements of the parameter distribution

The temperature profile of AB Dor is complex; previous fits used 3-temperature or EMD models

| Phot.# | $\lambda_{spec}(\text{\AA})$ | $\lambda_{sim}(\text{\AA})$ | $\log(T)$ | Type      |
|--------|------------------------------|-----------------------------|-----------|-----------|
| 1      | 18.990                       | 18.967                      | 6.796     | O VIII    |
| 2      | 12.903                       | 12.308                      | 6.839     | Continuum |
| 3      | 10.762                       | 10.849                      | 7.096     | Ni XXIII  |
| 4      | 12.806                       | 12.846                      | 7.129     | Fe XX     |
| 5      | 17.930                       | 18.037                      | 6.662     | Continuum |
| 6      | 12.238                       | 12.284                      | 7.030     | Fe XXI    |
| ⋮      | ⋮                            | ⋮                           | ⋮         | ⋮         |

AB Dor Emission Measure Distribution

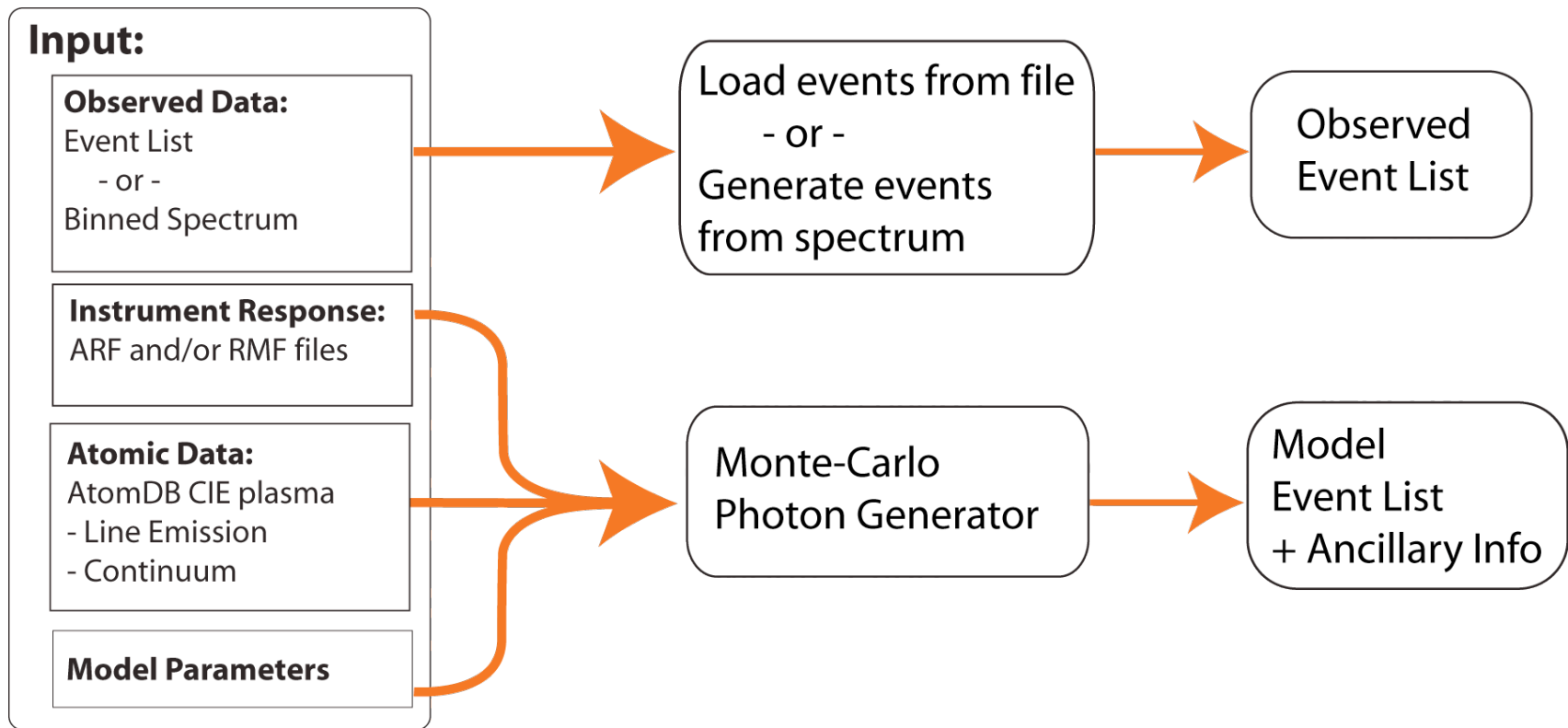


Histogram of PCM solution

Three vertical dashed lines are 3-T XSPEC fit from Sanz-Forcada, Maggio and Micela (2003)

# PCM Algorithm Progression

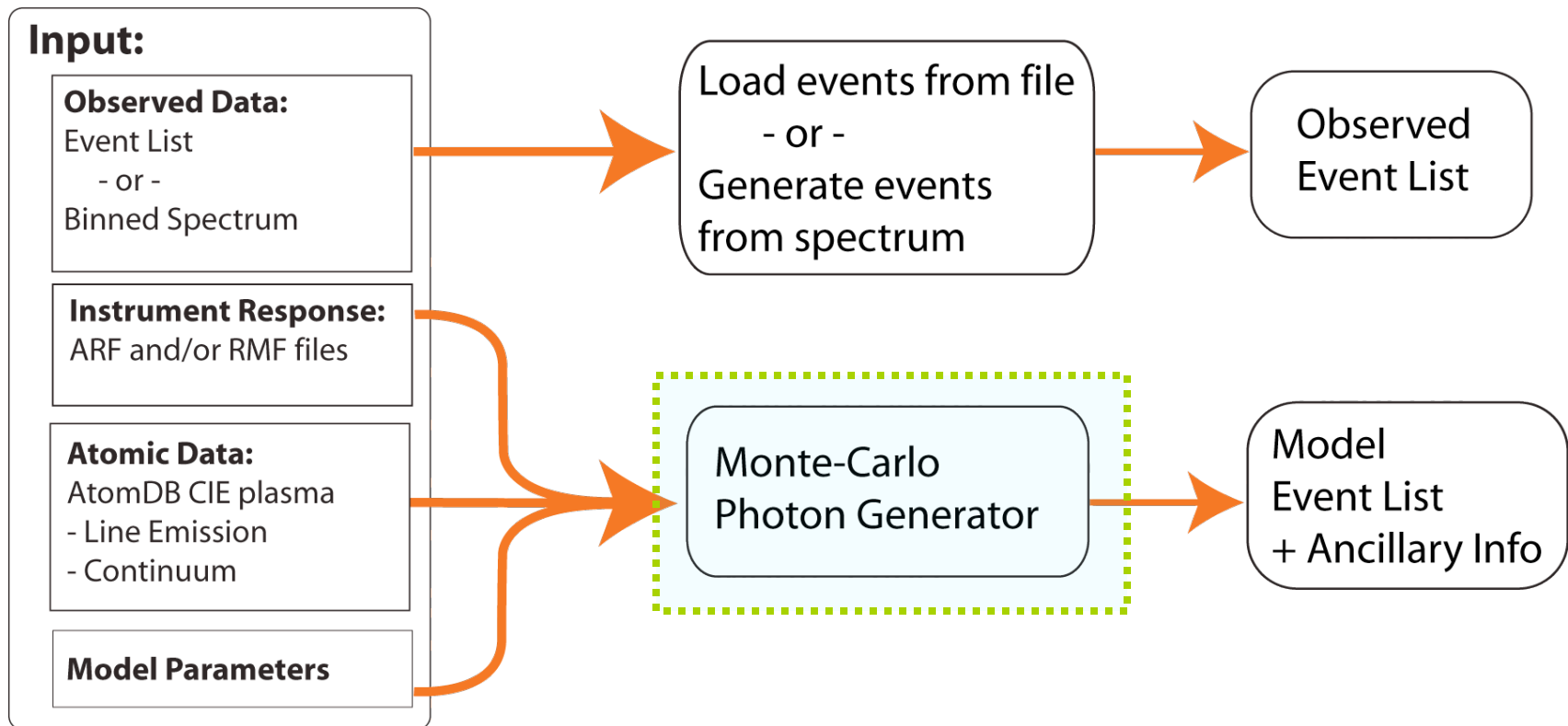
Start: Generate initial model + simulated detected photons from input parameter distribution





# PCM Algorithm Progression

Start: Generate initial model + simulated detected photons from input parameter distribution



# Photon Generator

Start: Model Parameter (T)

## For CIE Plasma:

- Given a temperature (T), AtomDB generates spectral energy (E).
- Apply ARF test to determine whether photon is detected
- If photon is detected, apply RMF to determine detected energy (E')

Model Data:  
AtomDB

ARF test

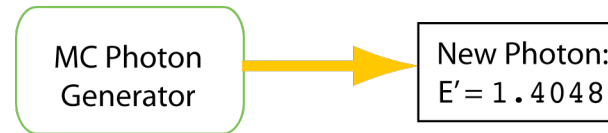
RMF Energy  
Redistribution

Result: (T,E,E')  
+ Ancillary Info

# PCM Algorithm: Iterate with Feedback

Iteration:

- Generate 1 detected photon



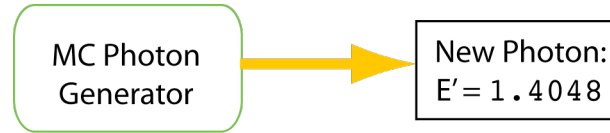
Model  $E_{\text{sim}}$

|        |
|--------|
| ⋮      |
| 2.4903 |
| 1.6309 |
| 0.9901 |
| 1.4052 |
| 1.1385 |
| 1.6027 |
| 3.7938 |
| 2.4429 |
| ⋮      |

# PCM Algorithm: Iterate with Feedback

Iteration:

- Generate 1 detected photon
- Replace 1 random photon from model with new photon ( $E, E', T$ )



Model  $E_{\text{sim}}$

|        |
|--------|
| ⋮      |
| 2.4903 |
| 1.6309 |
| 0.9901 |
| 1.4052 |
| 1.1385 |
| 1.6027 |
| 3.7938 |
| 2.4429 |
| ⋮      |

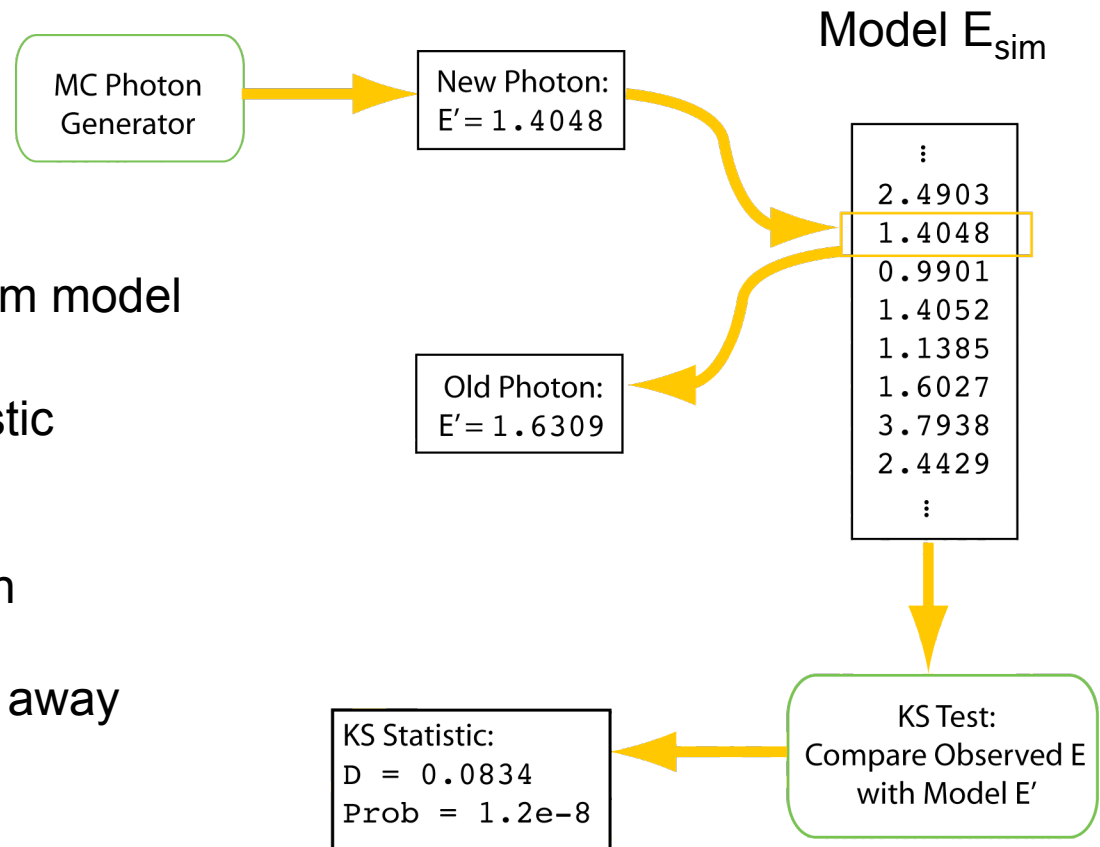
# PCM Algorithm: Iterate with Feedback

## Iteration:

- Generate 1 detected photon
- Replace 1 random photon from model with new photon ( $E, E', T$ )
- Compute KS probability statistic

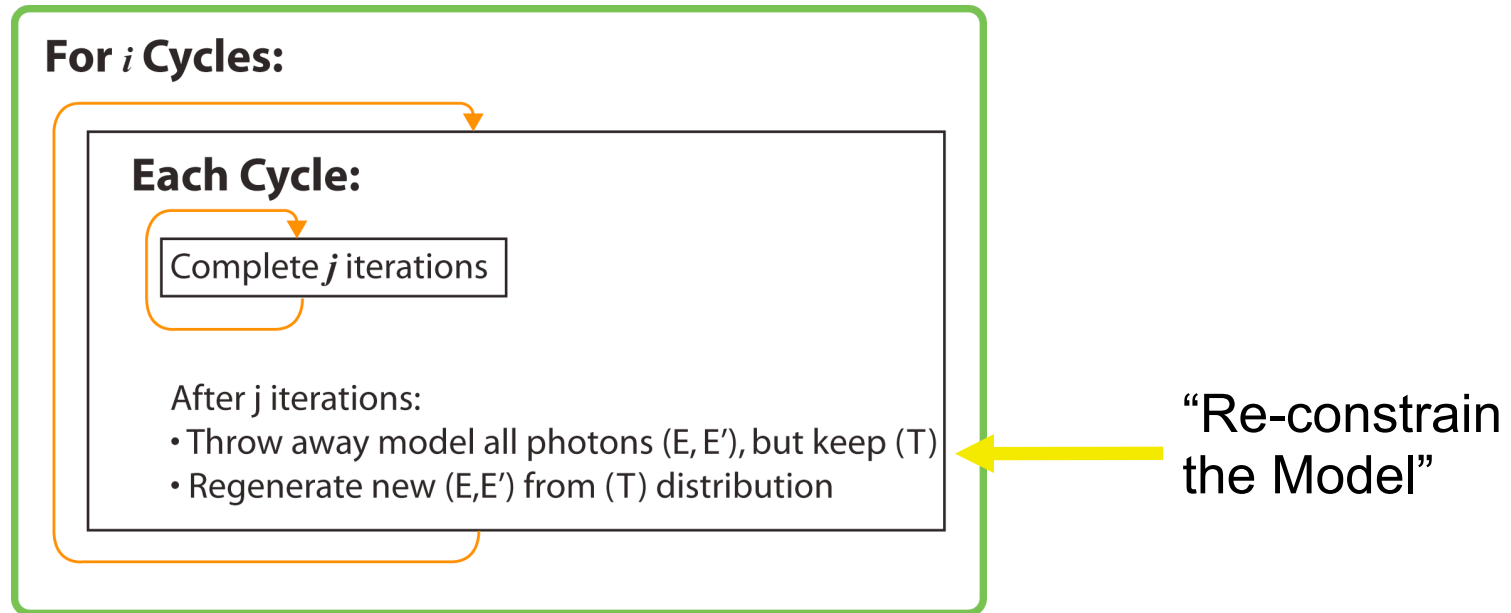
## Feedback Test:

If KS probability improves with new photon, keep it;  
 Otherwise, throw new photon away and keep old photon



# PCM Analysis Modes

## Phase I: Constrained Convergence

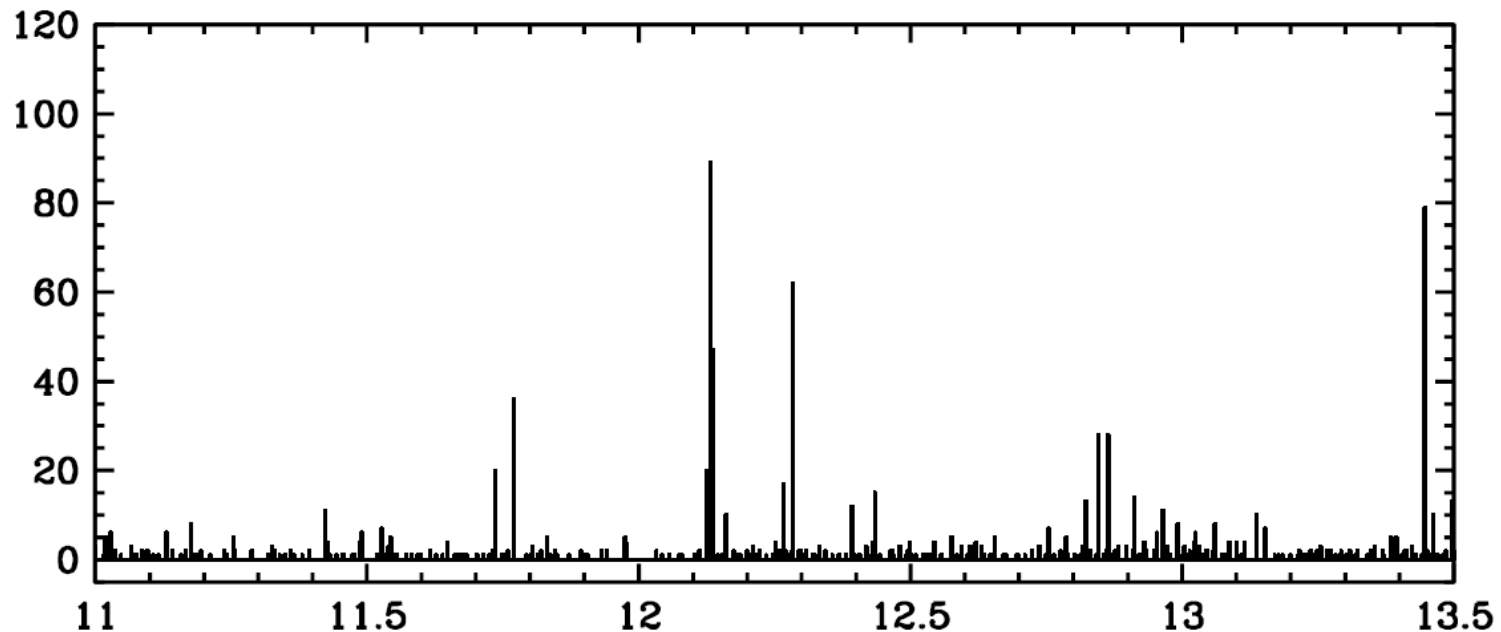


- Generates a solution which is consistent with a physically realizable model

# PCM Analysis Modes

## Phase II: Un-Constrained Convergence:

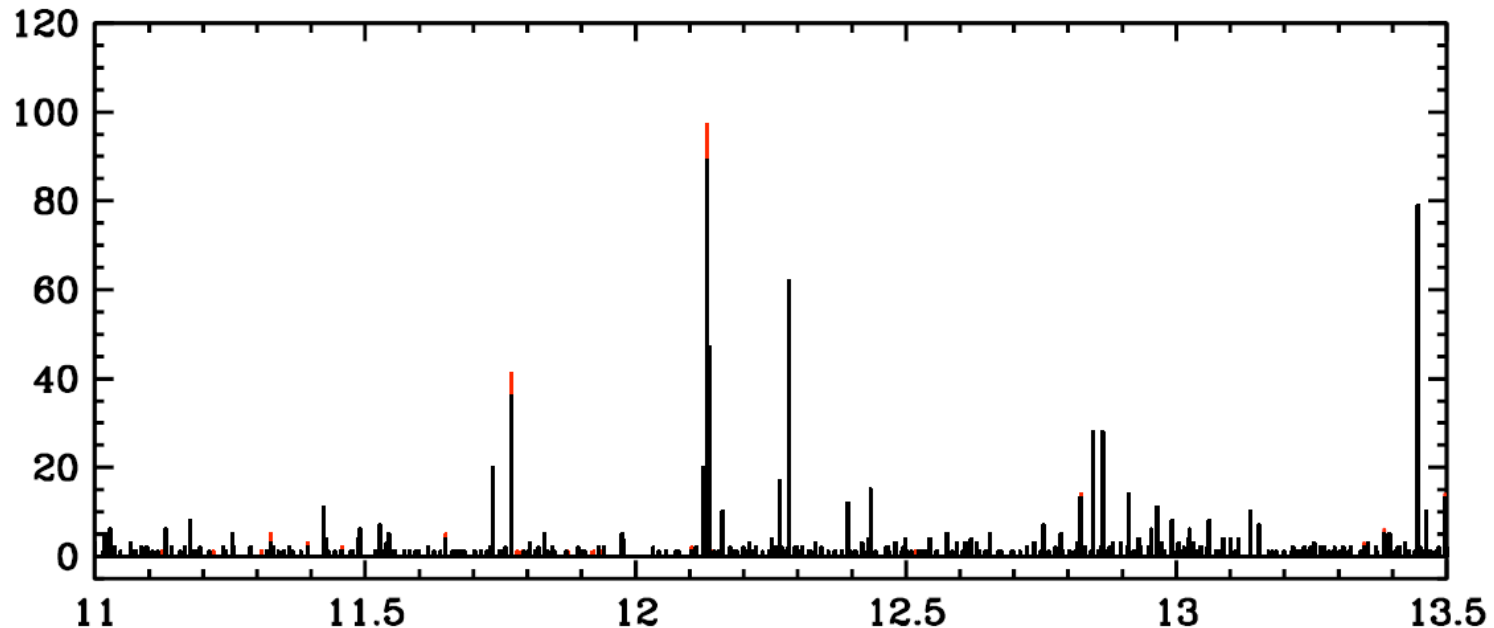
- Iterate until KS probability reaches cutoff value, with Monte-Carlo Markov Chain weighting
- Photon distribution is not constrained to model probabilities
- Allows individual spectral features to be modified to produce best-fit solution



# PCM Analysis Modes

## Phase II: Un-Constrained Convergence:

- Iterate until KS probability reaches cutoff value, with Monte-Carlo Markov Chain weighting
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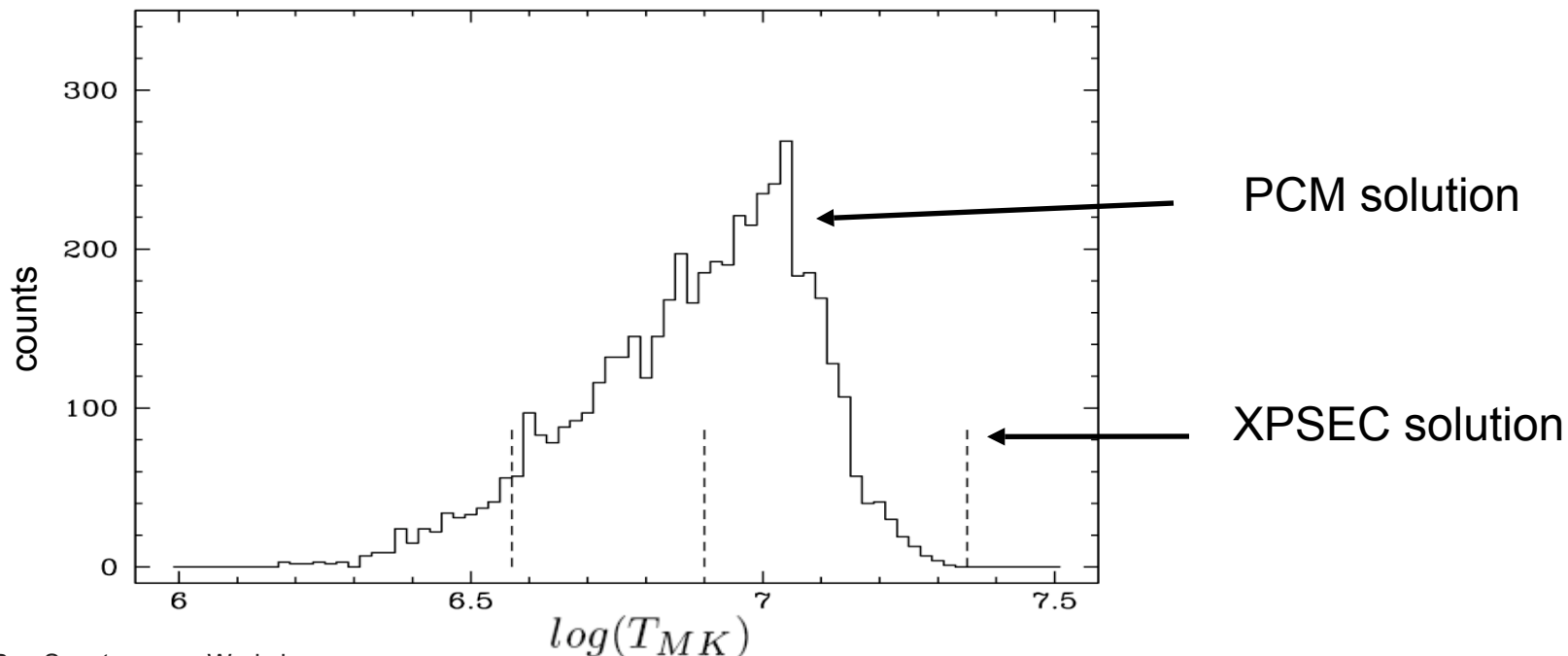


# Determining Variation in Many-Parameter Models

Low-dimensionality models with few degrees of freedom may be quantified using Chi-square test which has a well-defined error methodology. PCM is appropriate for models of high dimensionality where every photon is a free parameter.

For error determination we use distribution-driven re-sampling methods

⇒ Bootstrap Method



# Bootstrap Re-Sampling

---

## Method:

- 1) Randomly resample input data set with substitution to create new data set
- 2) Perform analysis on new data set to produce new outcome
- 3) Repeat for  $n \gg 1$  re-sampled data sets

# Bootstrap Re-Sampling

---

## Method:

- 1) Randomly resample input data set with substitution to create new data set
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15.020  
14.961  
7.622  
17.711  
21.549  
16.062  
14.376  
13.298  
12.833  
17.801

# Bootstrap Re-Sampling

## Method:

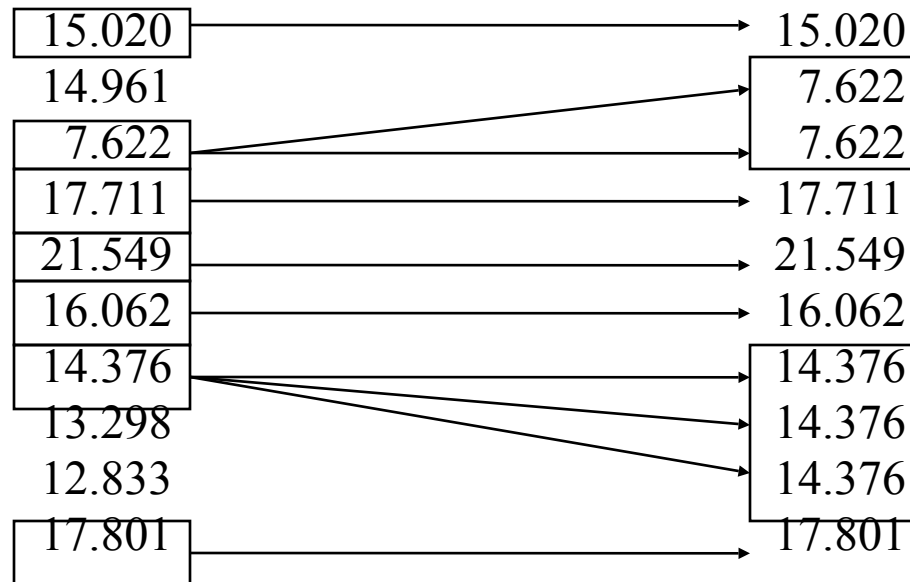
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|        |
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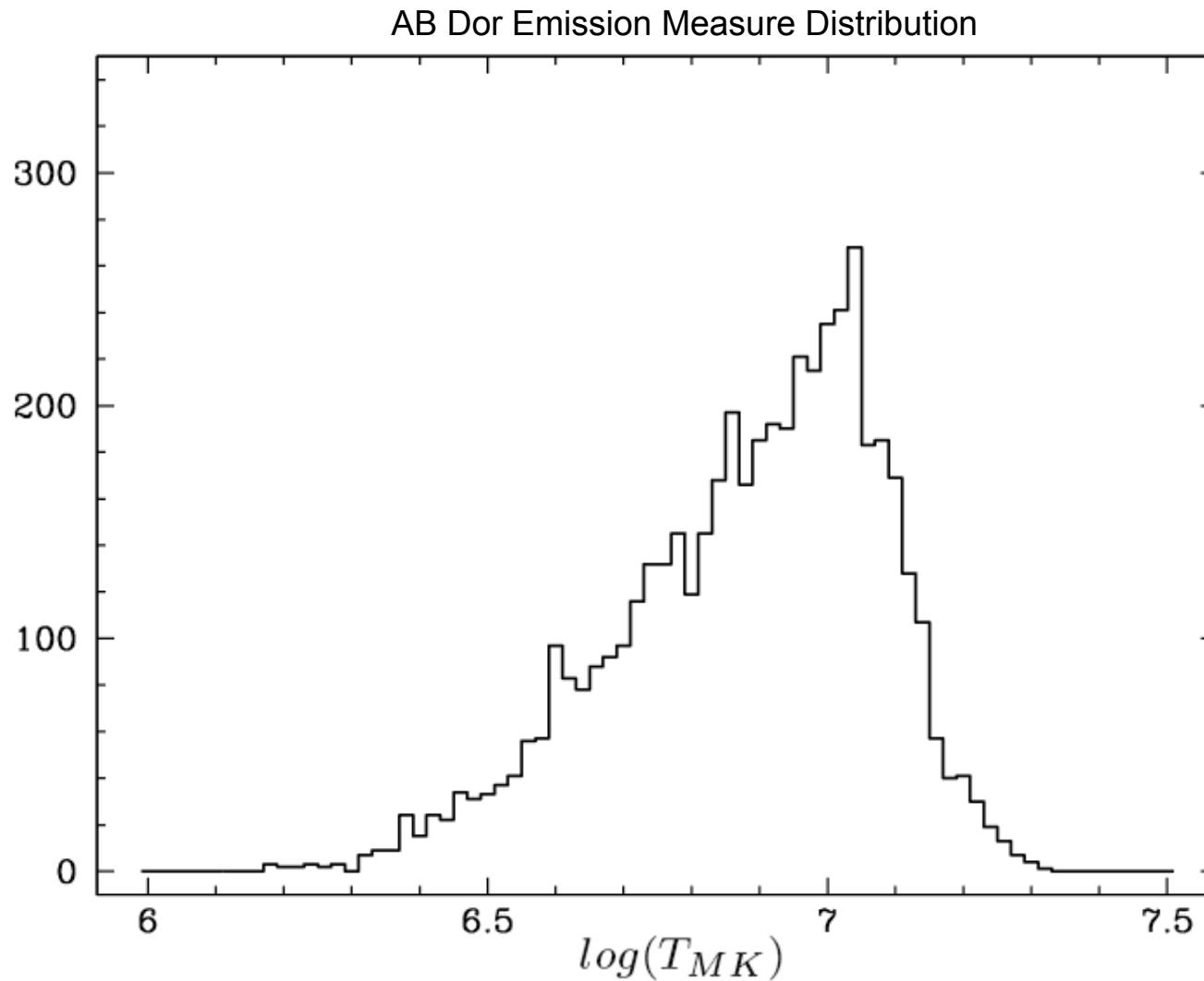
# Bootstrap Re-Sampling

Method:

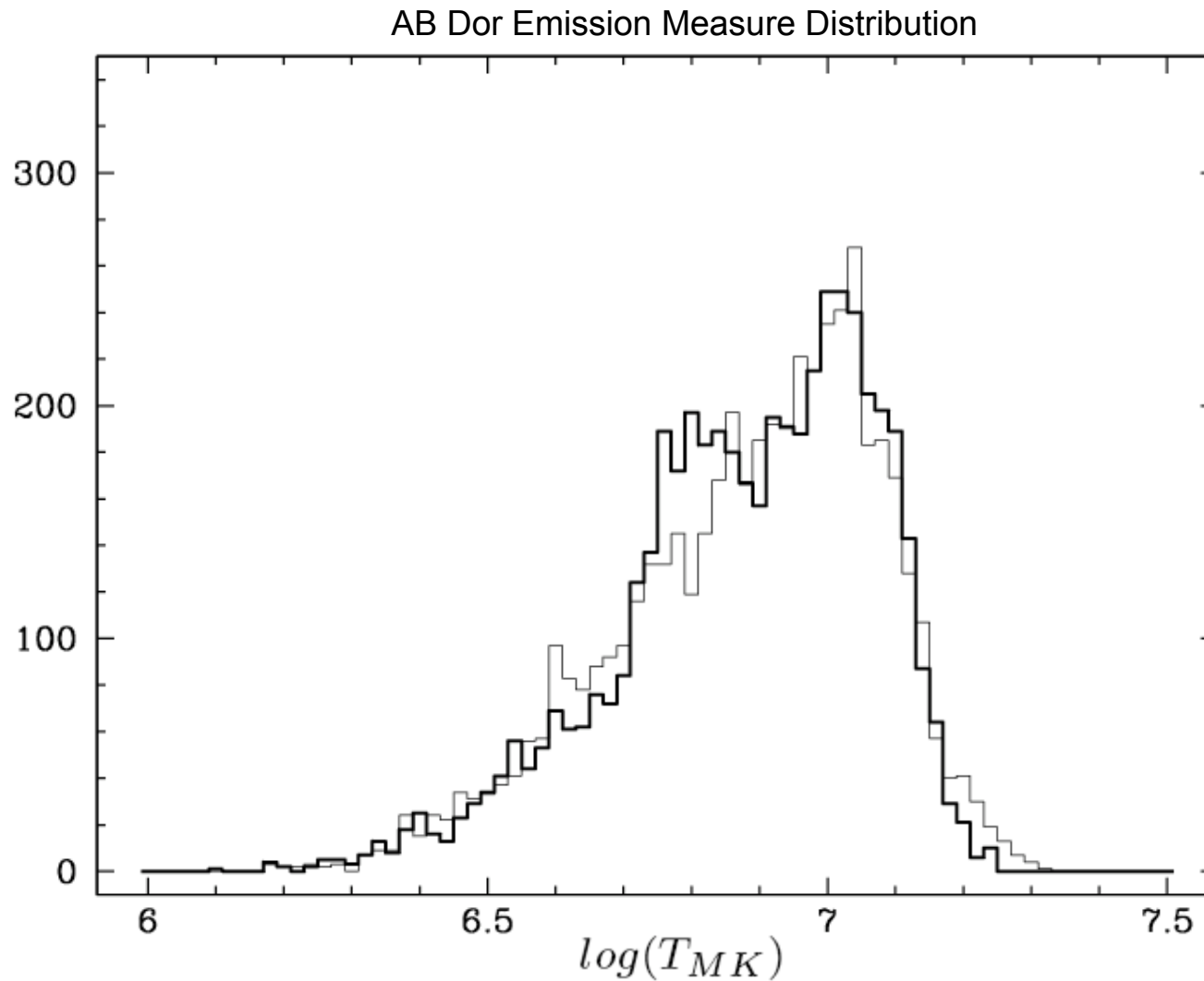
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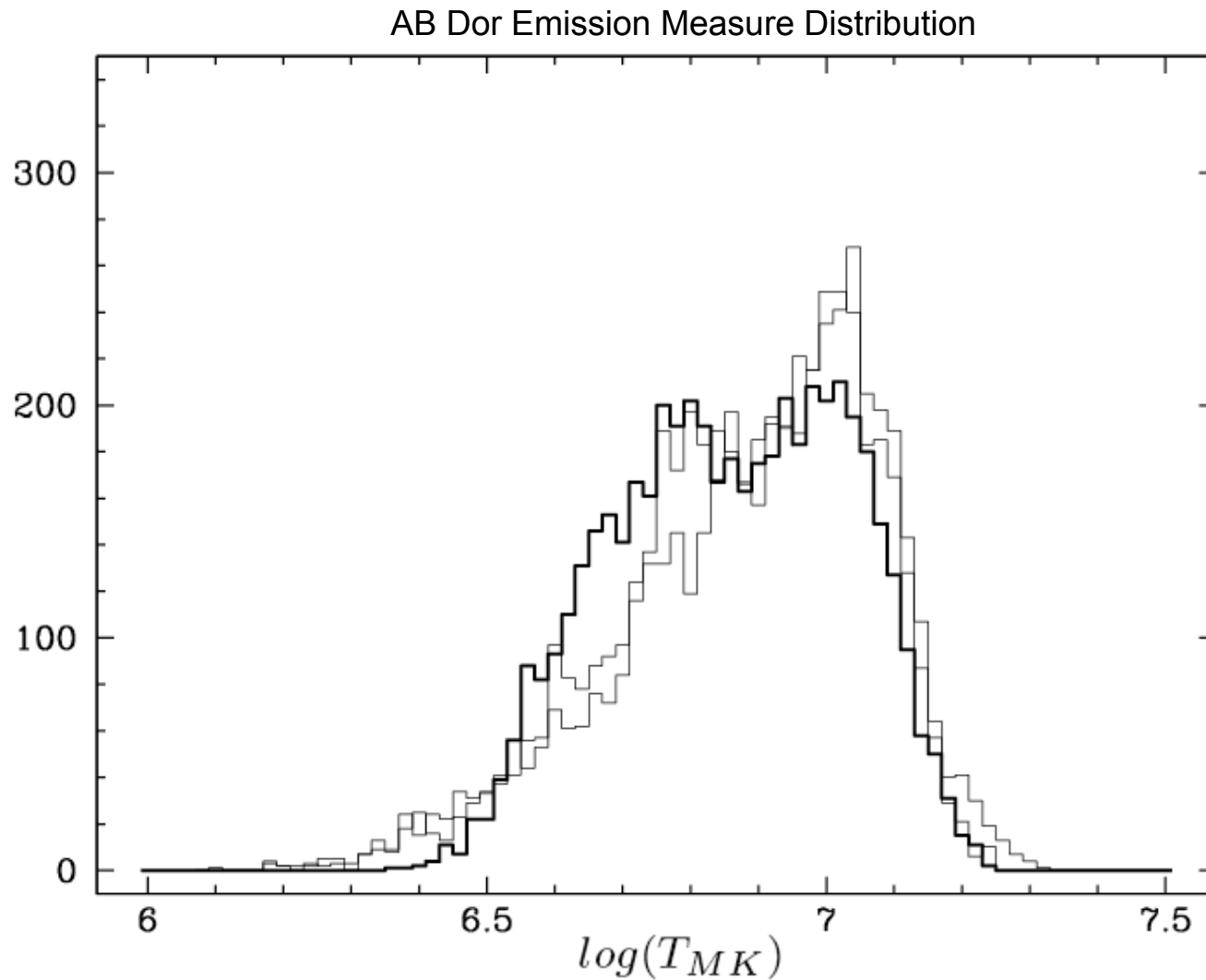
# Bootstrap Results



# Bootstrap Results

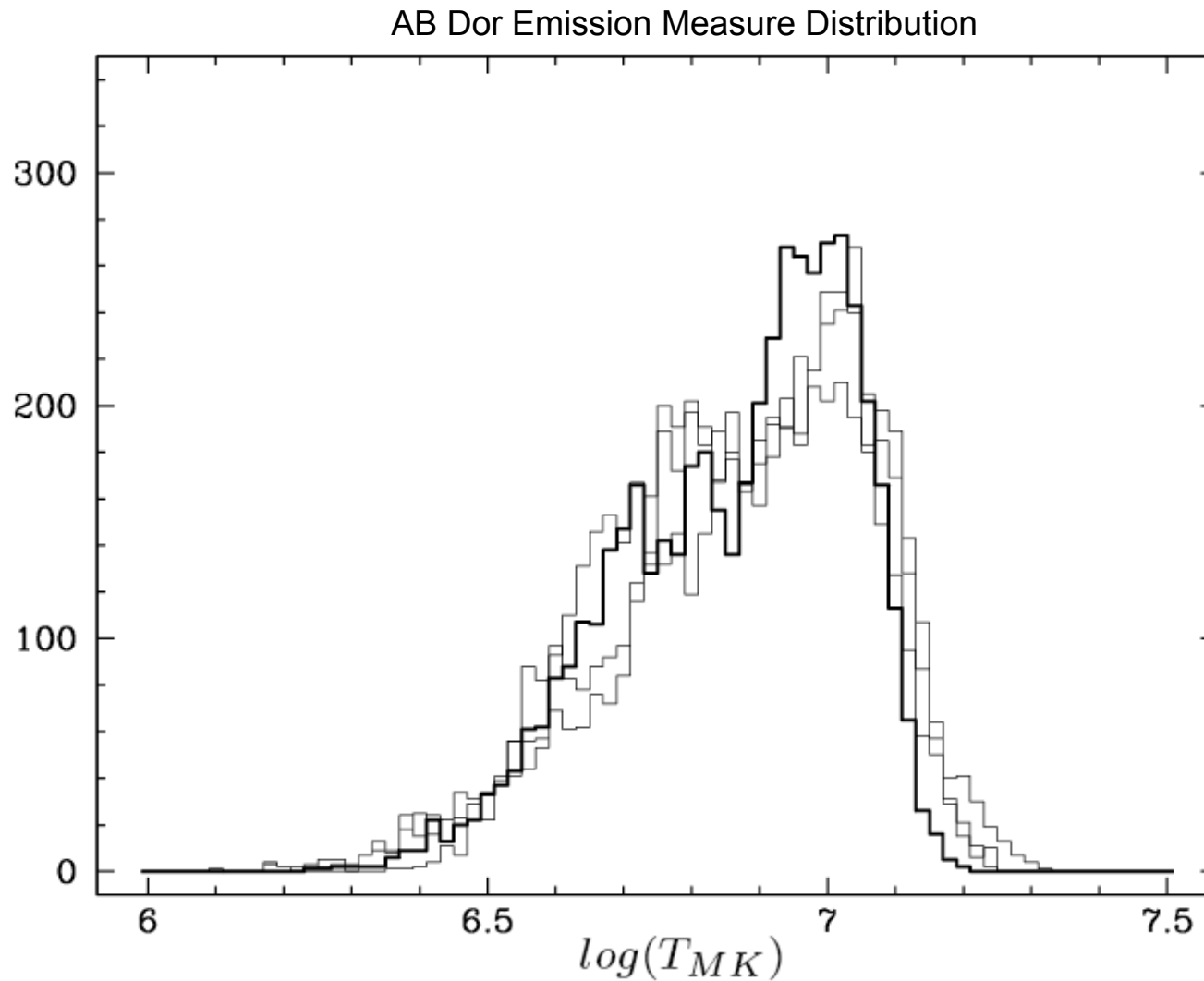


# Bootstrap Results

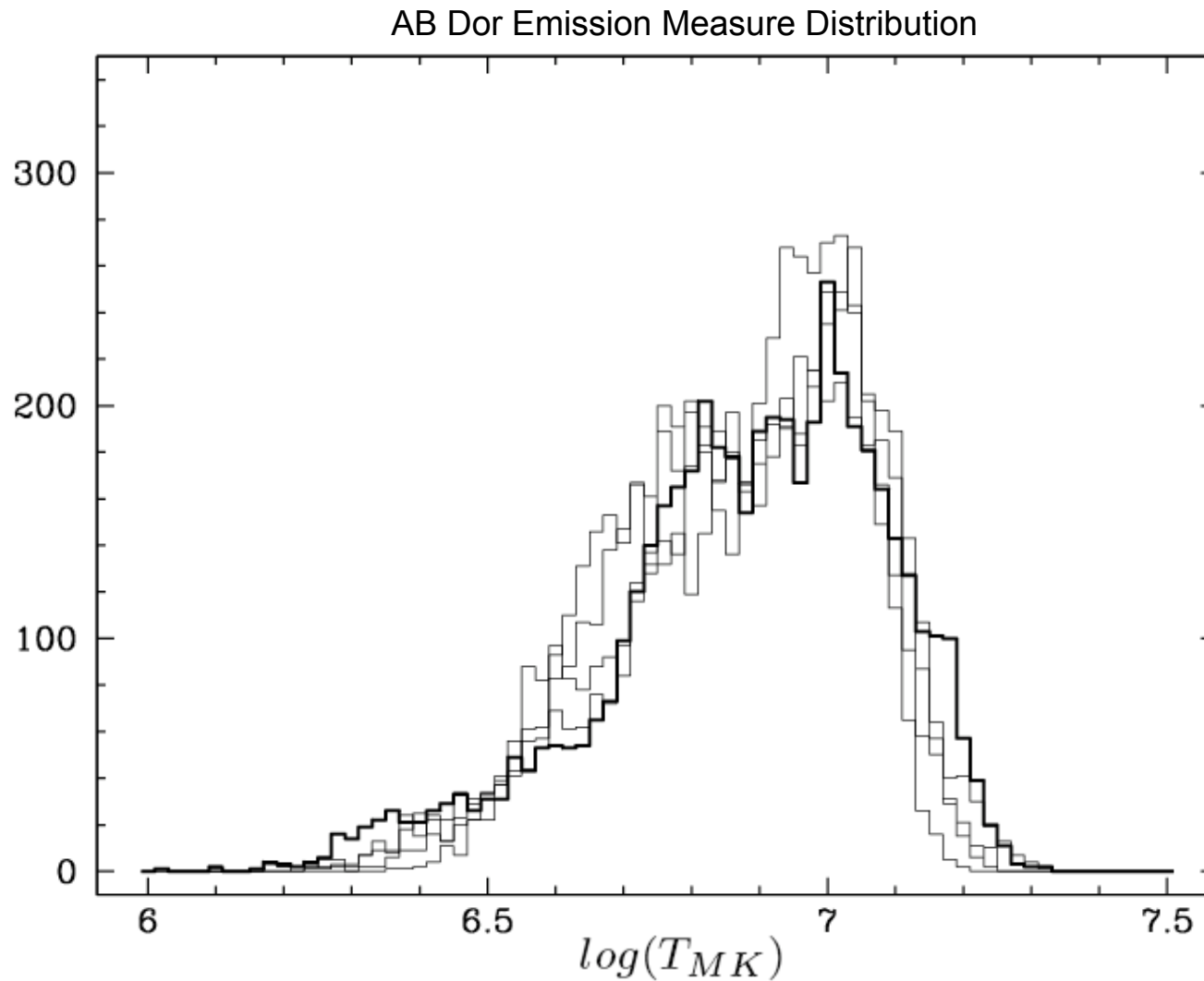




# Bootstrap Results



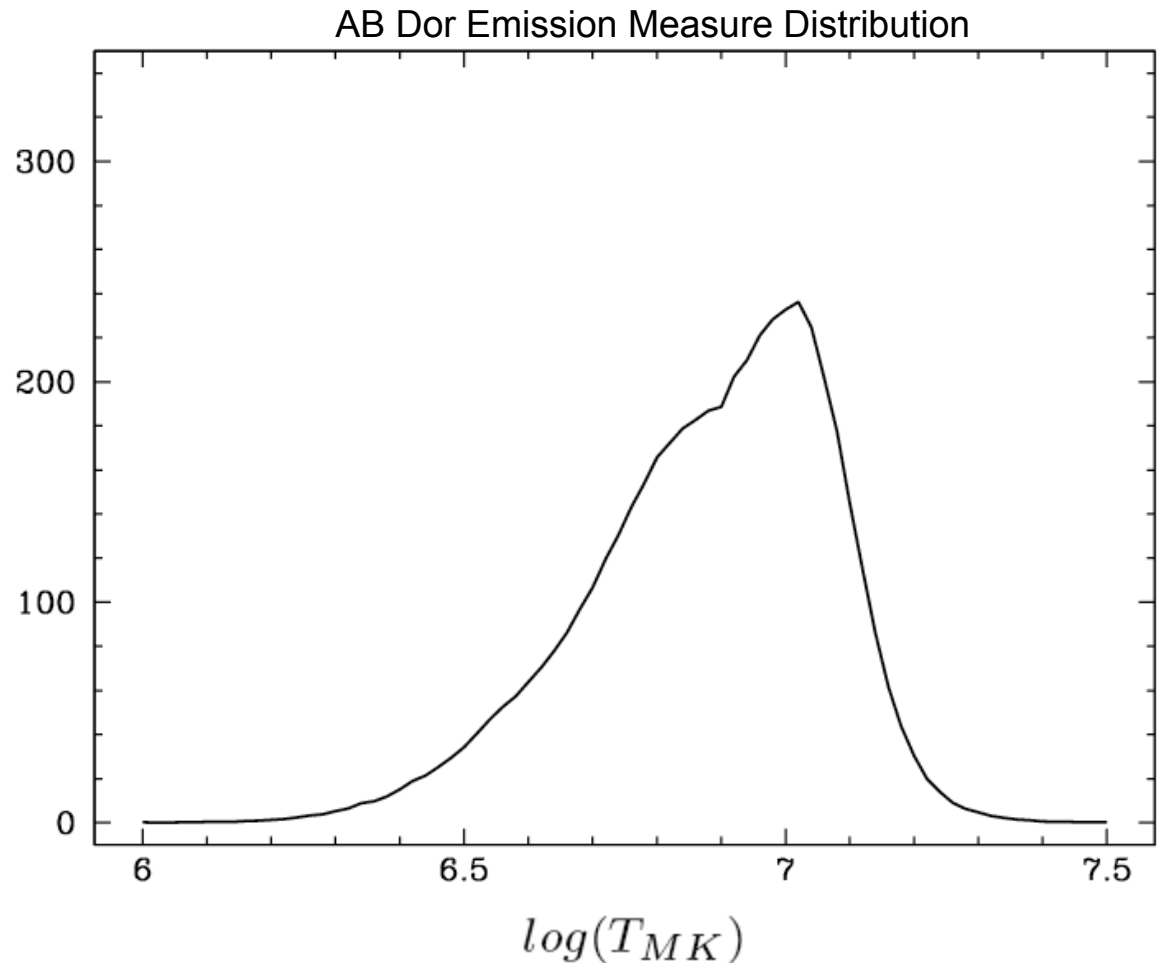
# Bootstrap Results



# Interpreting the Bootstrap

The variations in the bootstrap solutions estimate errors

The Arithmetic mean of all distributions is plotted as solid line

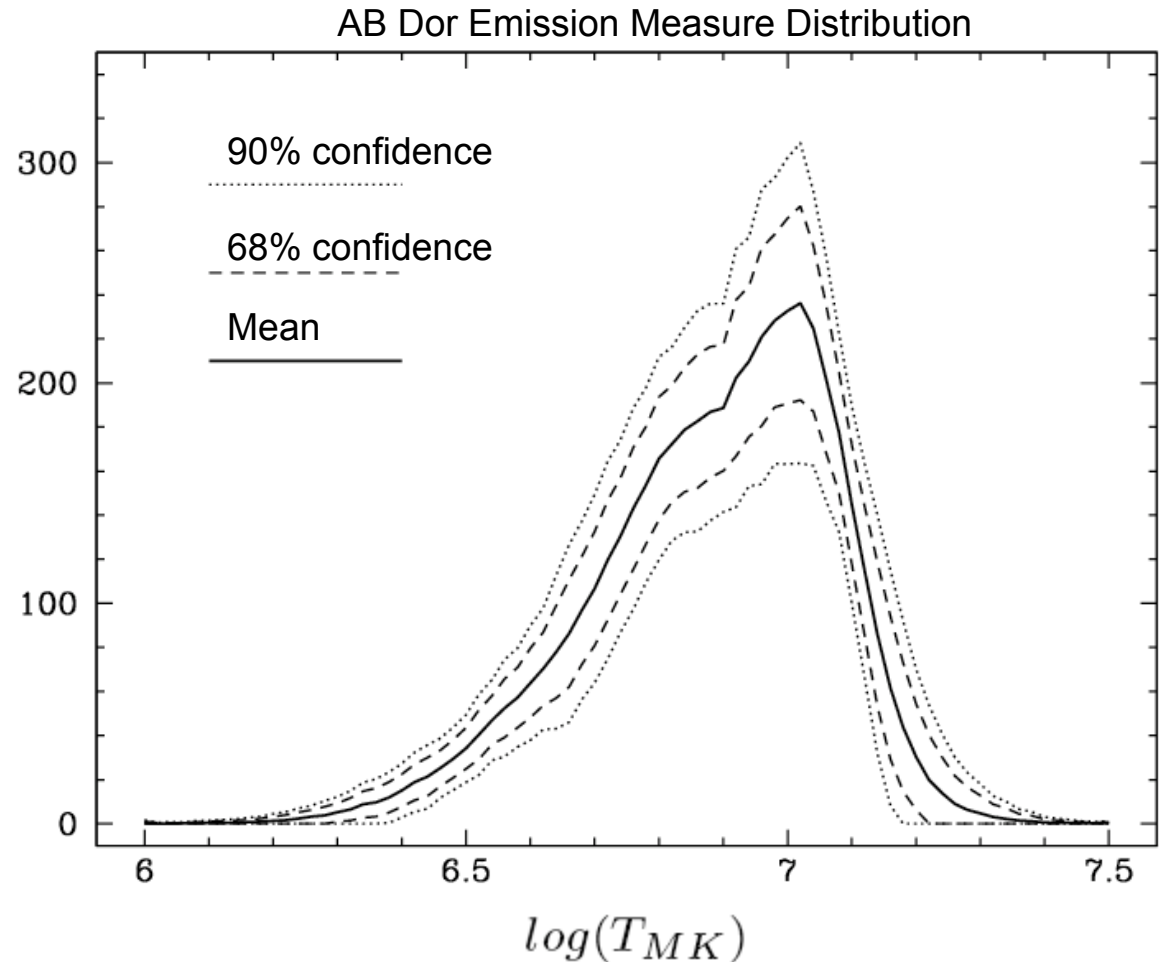


# Interpreting the Bootstrap

The variations in the bootstrap solutions estimate errors

The Arithmetic mean of all distributions is plotted as solid line

Confidence levels are computed along vertical axis of distribution



# Summary

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- The Photon Clean Method allows for complicated parameter distributions
- Phase I solution gives best-fit solution from existing models
- Phase II solution modifies model to quantify amount of departure from physical models
- Bootstrap re-sampling may determine variability of trivial and non-trivial solutions without assumptions about the underlying distribution of the data
- As a test of the PCM's ability to simultaneously model Fe K and Fe L shell line emission, we are using it to model spectra produced by the LLNL EBIT's Maxwellian plasma simulator mode.

**Thank You**