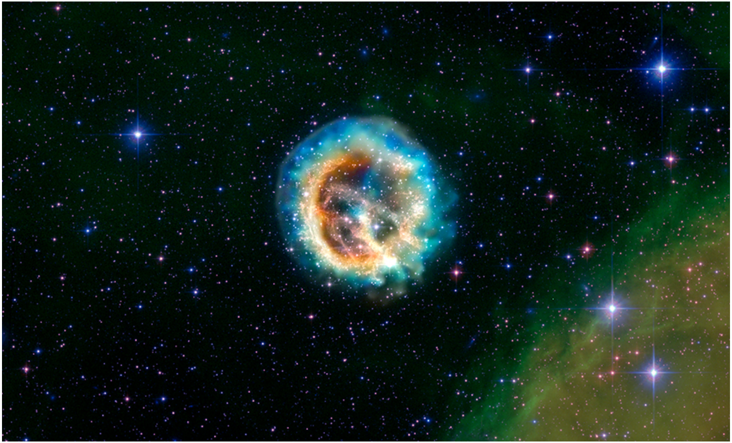
# Calibration Concordance for Astronomical Instruments

Yang Chen

Joint work with X.-L. Meng (Harvard University), X. Wang (Two Sigma Inc.), D. van Dyk (Imperial College London), V. Kashyap (Center for Astronomy), H. Marshall (MIT)

June 7, 2021

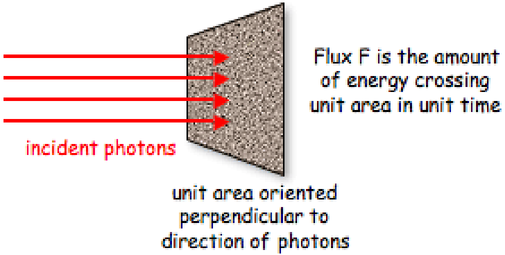
# Calibration Concordance Problem (Example: E0102)

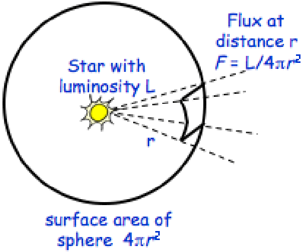


- Supernova remnant E0102
- Four sources correspond to four spectral lines in E0102

# Measurements

Flux is the total amount of energy that crosses a unit area per unit time.

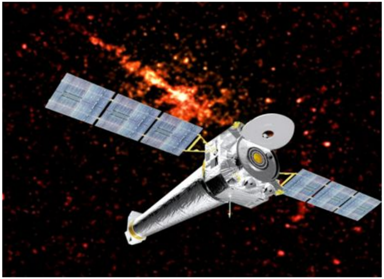



The flux of an astronomical source (F) depends on the luminosity of the object (L) and its distance from the Earth (r), $F = L/4\pi r^2$.

# Observatory and Instruments

## Current X-ray Observatory



USA: Chandra X-ray Observatory

High angular resolution (~0.5")

Europe: XMM-Newton

High throughput (large effective area)

And

- •Rossi X-ray Timing Explorer
- •Swift
- •INTEGRAL etc.

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# Observatory and Instruments

CHANDRA
X-RAY OBSERVATORY

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Instruments & Calibration | For the Public

## Chandra Instruments and Calibration

The Chandra X-ray Observatory (CXO) is designed for high resolution (≤ 1/2 arcsec) X-ray imaging and spectroscopy. The High Resolution Mirror Assembly (HRMA) focuses X-rays onto one of two instruments, ACIS or HRC. Only one detector (HRC or ACIS) is in the focal plane at any given time. Two grating spectrometers (LETG or HETG) can be placed in the optical path behind the HRMA. The dispersed spectrum is read out by either ACIS or HRC. A high level overview of the instruments on-board the Chandra X-ray Observatory can be found on the About Chandra pages and a more detailed description can be found in the Proposers' Observatory Guide.

Current calibration data products for use in CIAO and other analysis systems can be found in the CALDB pages. A complete listing of all calibration products in the CALDB and a brief description of these products can be found in the Calibration Data Products.

- Calibration Status Summary
- ACIS
- HRC
- HETG
- LETG
- HRMA
- Calibration Database (CALDB)
- Cross-Calibration with other X-Ray Telescopes
- Aspect Information
- Calibration Workshops and Reviews
- SPIE Proceedings
- Science and Calibration Requirements

### Advanced CCD Imaging Spectrometer (ACIS)

The ACIS has two arrays of CCDs, one (ACIS-I) optimized for imaging wide fields (16x16 arc minutes) the other (ACIS-S) optimized as a readout for the HETG transmission grating. One chip of the ACIS-S (S3) can also be used for on-axis (8x8 arc minutes) imaging and offers the best energy resolution of the ACIS system.

### High Resolution Camera (HRC)

The HRC comprises two micro-channel plate imaging detectors, and offers the highest spatial (<0.5 arc second) and temporal (16 msec) resolutions. The HRC-I has the largest field-of-view (31x31 arc minutes) available on Chandra. The HRC-S is most commonly used to read out the dispersed spectrum from the LETG.

### High Energy Transmission Grating (HETG)

The HETG is optimized for high-resolution spectroscopy of bright sources over the energy band 0.4-10 keV. It is most commonly used with ACIS-S. The resolving power ($E/\Delta E$) varies from ~800 at 1.5 keV to ~200 at 6 keV.

### Low Energy Transmission Grating (LETG)

The LETG provides the highest spectral resolving power ($E/\Delta E > 1000$) on Chandra at low energies (0.07 - 0.2 keV). The LETG/HRC-S combination is used extensively for high resolution spectroscopy of bright, soft sources such as stellar coronae, white dwarf atmospheres and cataclysmic variables.

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Each of these instruments has a different photon collection efficiency – Effective Area. Reflectivity and vignetting, among other effects, cause the geometric area of a telescope to be reduced to a smaller "effective area".

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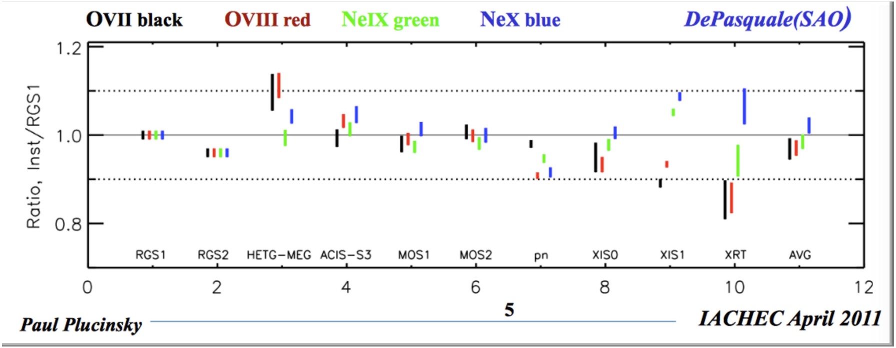


- Four spectral lines observed with 11 X-ray detectors
- Main challenge – the data/instruments do not agree

# Outline

1. Introduction
2. Scientific and Statistical Models
3. Concordance Model
4. Advantages of Our Approach
   - Multiplicative Shrinkages
   - Benefits of fitting the variances
   - Extentions to handle outliers
5. Results
6. Extensions
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- $N$ Instruments with true effective area $A_i$, $1 \leq i \leq N$.
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- Lower cases: data / estimators.
- Upper cases: parameter / estimand.

# Calibration Concordance Problem

1. Astronomers' Dilemma:

$$\frac{c_{ij}}{a_i} \neq \frac{c_{i'j}}{a_{i'}} \text{ for } i \neq i'.$$

Different instruments give different estimated flux of the same object!

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2. Scientific Question:

- Are there systematic errors in 'known' effective areas?
- Can we derive properly adjusted effective areas?
- Can we unify estimates of the same flux with different instruments?

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# Scientific and Statistical Models

## Scientific Model

Multiplicative in original scale and additive on the log scale.

$$\text{Counts} = \text{Exposure} \times \text{Effective Area} \times \text{Flux},$$
$$C_{ij} = T_{ij} A_i F_j, \quad \Leftrightarrow \quad \log C_{ij} = B_i + G_j,$$

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## Statistical Model

$$\text{log counts } y_{ij} = \log c_{ij} - \alpha_{ij} = B_i + G_j + e_{ij}, \quad e_{ij} \overset{indep}{\sim} \mathcal{N}(0, \sigma_{ij}^2);$$

where $\alpha_{ij} = -0.5\sigma_{ij}^2$ to ensure $E(c_{ij}) = C_{ij} = A_i F_j$.

- **Known Variances**: $\sigma_{ij}$ known.
- **Unknown Variances**: $\sigma_{ij} = \sigma_i$ unknown.

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# Bayesian Hierarchical Model

**Log-Normal Hierarchical Model.**

$$\begin{aligned} \text{log counts } | \textit{area} \,\&\, \textit{flux} \,\&\, \textit{variance} \quad &\overset{\text{indep}}{\sim} \quad \text{Gaussian distribution}, \\ y_{ij} \mid B_i,\ G_j,\ \sigma_i^2 \quad &\overset{\text{indep}}{\sim} \quad \mathcal{N}\left(B_i + G_j,\ \sigma_i^2\right), \end{aligned}$$

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**Setting the prior parameters.**

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**Setting the prior parameters.**

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# Bayesian Computation (Unknown Variances)

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- Hamiltonian Monte Carlo (HMC) – Stan package.
  - Highly correlated parameters, high-dim parameter space.

# Example Posterior Distributions

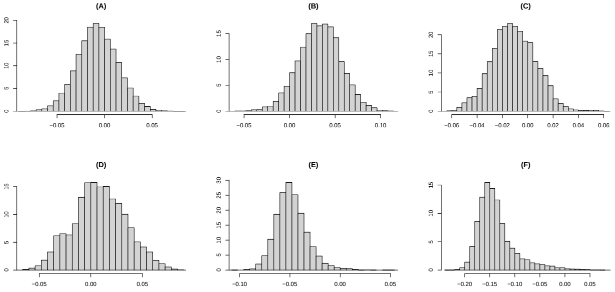


Figure 1: Posterior histograms for the fractional variation of the effective area. The data sets are (A) 2XMM data, hard band, XMM/pn, correlated $\tau$ values; (B) 2XMM data, hard band, XMM/MOS2, heterogeneous $\tau$ values; (C) XCAL data, medium band, XMM/pn, correlated $\tau$ values; (D) XCAL data, soft band, XMM/MOS1, $\tau = 0.05$ for all instruments; (E) 1E0102 data, O lines, Chandra/ACIS-S3, $\tau = 0.025$ for all instruments; and (F) 1E0102 data, O lines, Swift XRT/PC, $\tau = 0.05$ for all instruments.

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# Shrinkage Estimators: Known Fluxes and Errors

Hierarchical model $\Rightarrow$ Shrinkage estimators (weighted averages of evidence from 'Prior' and evidence from 'Data').

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Hierarchical model ⇒ Shrinkage estimators (weighted averages of evidence from 'Prior' and evidence from 'Data').

(1) When fluxes and variances are known,

## Original Scale

$$\hat{A}_i = a_i^{W_i} \left[ (\tilde{c}_{i\cdot} \tilde{f}^{-1}) e^{\sigma_i^2/2} \right]^{1-W_i},$$

where

$$\tilde{c}_{i\cdot} = \prod_j c_{ij}^{1/M}, \ \tilde{f} = \prod_j f_j^{1/M}$$

are geometric means.

## Log-Scale

$$\hat{B}_i = W_i b_i + (1 - W_i)(\bar{y}_{i\cdot} - \bar{G}),$$

where

$$\bar{G} = \frac{\sum_j g_j}{M}, \bar{y}_{i\cdot} = \frac{\sum_j y_{ij}}{M}$$

are arithmatic means.

The 'weights', $W_i = \frac{\tau_i^{-2}}{\tau_i^{-2} + M\sigma_i^{-2}}$, represents the direct information in $b_i$ relative to indirect information in fluxes.

# Shrinkage Estimators: Known Errors

(2) When fluxes are unknown and variances are known,

$$\hat{B}_i = W_i b_i + (1 - W_i)(\bar{y}_{i\cdot} - \bar{G}_i), \quad \hat{G}_j = \bar{y}_{\cdot j} - \bar{B},$$

where $\bar{G}_i = \frac{\sum_j \hat{G}_j}{M}, \quad \bar{B} = \frac{\sum_i \hat{B}_i \sigma_i^{-2}}{\sum_i \sigma_i^{-2}}, \bar{y}_{i\cdot} = \frac{\sum_j y_{ij}}{M}, \quad \bar{y}_{\cdot j} = \frac{\sum_i y_{ij} \sigma_i^{-2}}{\sum_i \sigma_i^{-2}}.$

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(3) When variances are unknown, shrinkage estimator of variance,

$$\hat{\sigma}_i^2 = \frac{2}{1 + \sqrt{1 + S_{y,i}^2}} \, S_{y,i}^2, \quad S_{y,i}^2 = \frac{1}{|J_i| + \alpha} \left[ \sum_{j \in J_i} (y_{ij} - \hat{B}_i - \hat{G}_j)^2 + \beta \right]$$

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    $\Rightarrow$ possible false discoveries
  - 'known variances' $\geq$ true variability

    $\Rightarrow$ noninformative results

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# Extentions: Log-t Model

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If $\xi_{ij} \overset{\text{indep}}{\sim} \chi^2_\nu$, i.e. independent chi-squared distributions, the error term

$Z_{ij}/\sqrt{\xi_{ij}}$ follows independent student-t distributions, i.e. $\frac{Z_{ij}}{\sqrt{\xi_{ij}}} \overset{\text{indep}}{\sim} \frac{\sigma}{\sqrt{\nu}} \mathrm{t}_\nu$.

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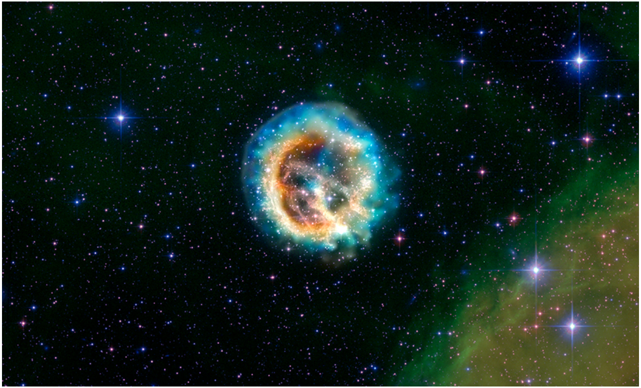
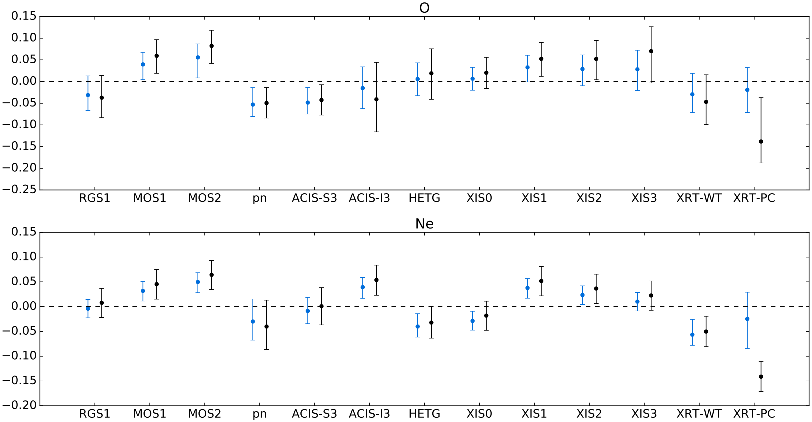
# Numerical Results (E0102)

**Recap**: Supernova remnant E0102.

Four sources are four spectral lines in E0102.



# Estimates of $B_i = \log A_i$ ($M = 2$ each panel)




- Adjusted so that default effective area, $b_i = \log a_i = 0$.
- 95% posterior intervals (black:$\tau = 0.05$; blue: $\tau = 0.025$).
- Some instruments systematically high, others low.

# Prior Influence

| Instrument | Oxygen | | Neon | |
|---|---|---|---|---|
| | $\tau = 0.025$ | $\tau = 0.05$ | $\tau = 0.025$ | $\tau = 0.05$ |
| RGS1 | 0.570 | 0.205 | 0.063 | 0.016 |
| MOS1 | 0.279 | 0.077 | 0.075 | 0.019 |
| MOS2 | 0.355 | 0.065 | 0.077 | 0.017 |
| pn | 0.250 | 0.041 | 0.620 | 0.218 |
| ACIS-S3 | 0.218 | 0.040 | 0.270 | 0.088 |
| ACIS-I3 | 0.906 | 0.640 | 0.099 | 0.026 |
| HETG | 0.648 | 0.341 | 0.129 | 0.034 |
| XIS0 | 0.180 | 0.051 | 0.069 | 0.018 |
| XIS1 | 0.298 | 0.078 | 0.071 | 0.019 |
| XIS2 | 0.463 | 0.140 | 0.063 | 0.016 |
| XIS3 | 0.772 | 0.364 | 0.062 | 0.018 |
| XRT-WT | 0.726 | 0.278 | 0.154 | 0.026 |
| XRT-PC | 0.934 | 0.235 | 0.906 | 0.017 |

Table 1: Proportion of prior influence, as defined by $1 - W_i$, for E0102 data.

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- Three EPIC instruments: the EPIC-pn, and the two EPIC-MOS detectors (pn, MOS1, and MOS2).
- Three datasets: hard (2.5 - 10.0 keV), medium (1.5 - 2.5 keV) and soft (0.5 - 1.5 keV) energy bands. The three instruments (pn, MOS1 and MOS2) measured 41, 41, and 42 sources respectively in hard, medium, and soft bands. Faint sources.

# Numerical Results (2XMM)

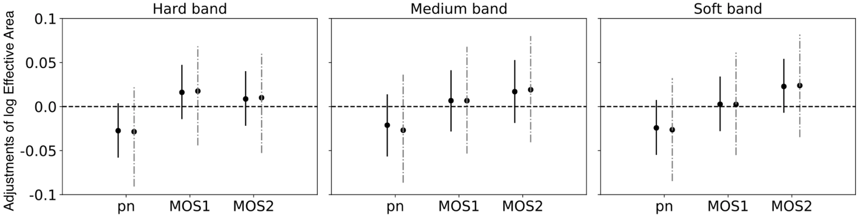



Figure 2: Adjustments of the log-scale Effective Areas for hard band (left), medium band (middle) and soft band (right) of the 2XMM datasets.

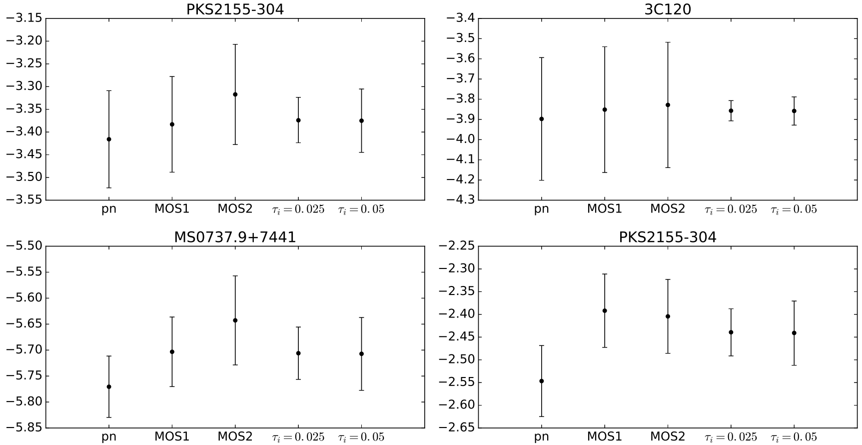
# Numerical Results (XCAL)

- **XCAL data**: Bright active galactic nuclei from the XMM-Newton cross-calibration sample.
  - Observed in hard ($n = 94$), medium ($n = 103$), soft ($n = 108$) bands.
- **Pileup**: Image data are clipped to eliminate the regions affected by pileup, determined using `epatplot`.
- **Three detectors**: MOS1, MOS2 and pn.
- We fit our model and show results on

**Sources**: M=103 (in medium band).

The hard and soft bands data are fitted similarly – treating hard/medium/soft band as three different data sets.

# Numerical Results (XCAL): Calibration Concordance




4 out of 103 Sources in medium band. y-axis: $G$ (log flux); vertical bars (left 3 in each panel): mean $\pm$ 2 s.d. based on observed fluxes, vertical bars (right 2 in each panel): 95% posterior intervals based on our model.

# Prior Influence

| Data Name | $\tau_i = 0.025$ | | | $\tau_i = 0.05$ | | |
|---|---|---|---|---|---|---|
| | pn | mos1 | mos2 | pn | mos1 | mos2 |
| hard band 2XMM | 0.093 | 0.075 | 0.082 | 0.025 | 0.020 | 0.022 |
| medium band 2XMM | 0.250 | 0.216 | 0.222 | 0.076 | 0.065 | 0.067 |
| soft band 2XMM | 0.093 | 0.075 | 0.069 | 0.025 | 0.020 | 0.018 |
| hard band XCAL | 0.010 | 0.019 | 0.031 | 0.003 | 0.005 | 0.008 |
| medium band XCAL | 0.023 | 0.016 | 0.028 | 0.006 | 0.004 | 0.007 |
| soft band XCAL | 0.021 | 0.011 | 0.007 | 0.005 | 0.003 | 0.002 |

Table 2: Proportion of prior influence.

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# Extensions to Account for Correlated Energy Bands

## Heterogeneous Uncertainties in Effective Area Priors

- Instrument specific fractional uncertainty $\tau_i$

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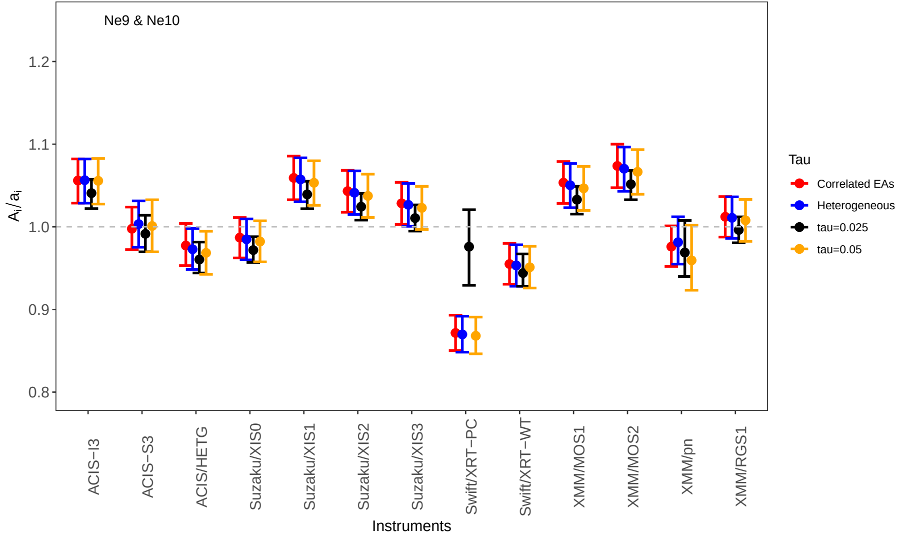
### Heterogeneous Uncertainties in Effective Area Priors

- Instrument specific fractional uncertainty $\tau_i$

### Correlations between Effective Area Priors

- allow correlations between the effective areas in different energy bands, which are taken as different "instruments" in the previous setup, for each instrument
- Correlations calculated based on Monte Carlo methods

# Extensions to Account for Correlated Energy Bands



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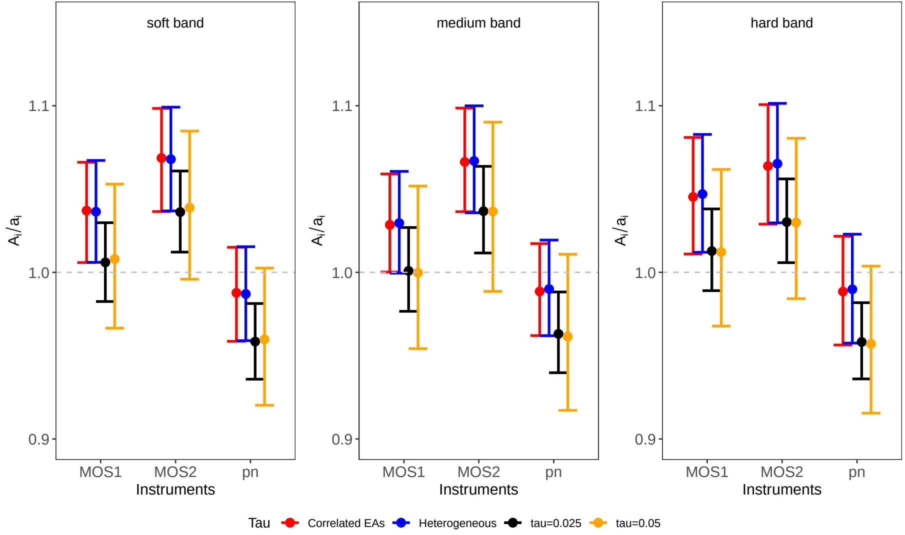

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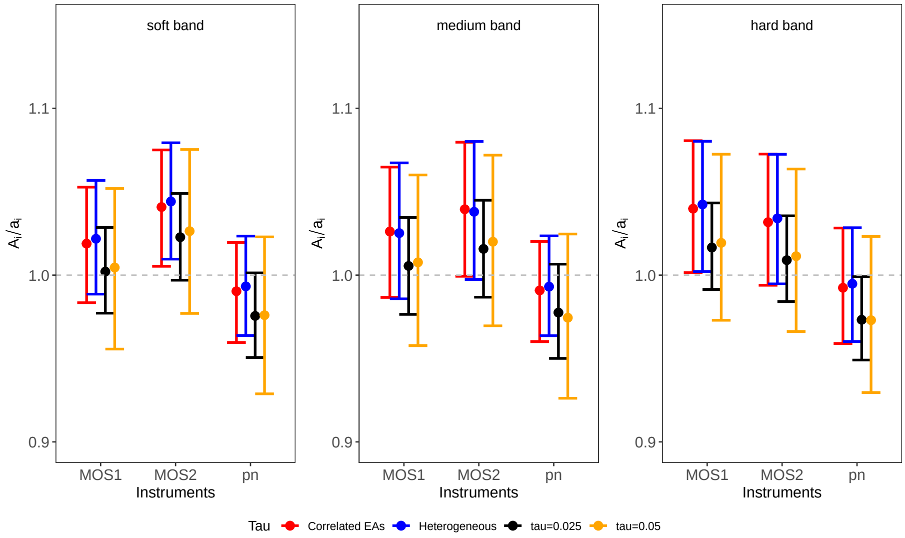

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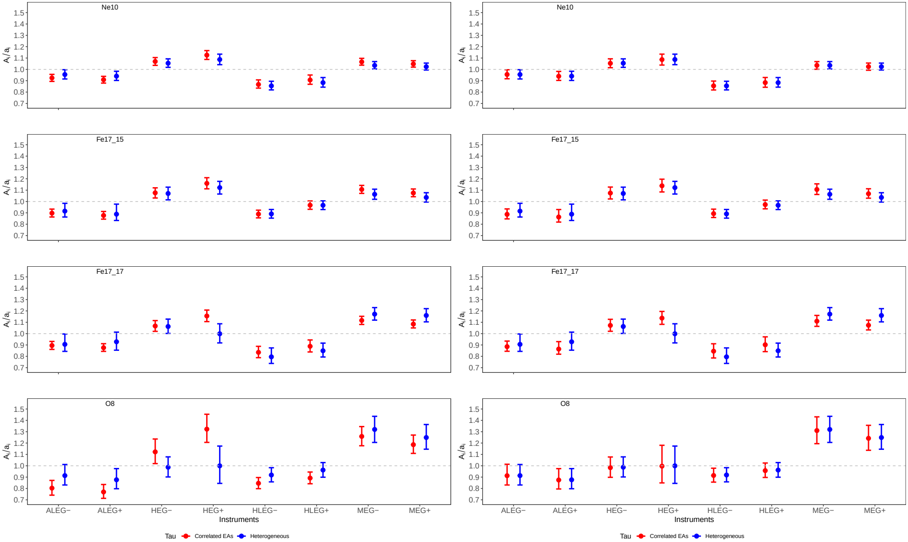

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2. Calibration concordance.

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