

Monte Carlo methods for including calibration uncertainties in model fitting analyses

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Jeremy J. Drake^a, Peter Ratzlaff^a, Vinay Kashyap^a and the Chandra MC Uncertainties Team
^aSmithsonian Astrophysical Observatory, Cambridge MA 02138

SUMMARY

- Instrument response uncertainties are complex and correlated, and almost universally ignored in astrophysical X-ray data analyses. For good quality observations, instrument response can be dominant source of error.
- We have developed Monte Carlo methods to treat calibration uncertainties for the Chandra ACIS. Here we calculate code and ancillary data will be released to Chandra Users. CIAO Skyrds methods are also under development to utilize these techniques (see accompanying poster by Kashyap et al).

Main Uncertainties in Instrument Response: Chandra ACIS-S

- HRMA: Geometry, Obscurability, Reflectivity, Scattering
- ACIS OBF: Transparency, Contamination, Uniformity
- ACIS CCD: Gain, Dark, Pulse Height Distribution

METHODS

Construct different realizations of instrument response by a combination of (1) randomly varying input parameters describing subassembly performance and (2) random multiplicative perturbation functions, $\mu(E)$, designed to sample subassembly responses with their assessed uncertainties (Fig. 1). Adopt "curtailed Gaussian" probability distribution $P(\sigma)$ for Monte Carlo draws (Fig. 1a). The different subassemblies were treated as follows:

HRMA On-Axis: Combination of perturbation functions, $\mu_{off}(E)$, and eyebox derived effective areas sampling the effects of different hydrocarbon contamination layers and interpretations of XRCF measurements (Figs. 2.3.4).

HRMA Vignetting Function: For off-axis angle θ (in arcmin), include fractional uncertainty of vignetting function, $V(\theta)$, and Debye-Waller related function.

ACIS OBF and Contamination Layer: OBF uses perturbation functions, $\mu_{OBF}(E)$, constrained by different allowed maximum deviations and relative edge discontinuities. The contamination perturbation function is:

$$\mu_{OBF}(E) = e^{-\mu_{OBF}(E) - \mu_{cont}(E) - \mu_{trans}(E) - \mu_{unif}(E)}$$

where σ_{OBF} , σ_{cont} , σ_{trans} and σ_{unif} are the fractional uncertainties in the optical depths C, O, F and Fluorine at a fiducial date (2003.29).

ACIS QE: combination of perturbation functions, $\mu_{QE}(E)$ and ACIS QE model predictions for uncertainties of 13% in CCD depletion depth and 20% in SiO₂ thickness.

ACIS Gain and Pulse Height Distribution: Uses RMFs generated for $P(\sigma_{gain})$ variations in gain and pulse height width; $\sigma_{gain} = 1\%$, 0.07 keV, 0.5% , 0.15 keV, and 0.2% , 0.2 keV.

ESTIMATING EFFECTS OF CALIBRATION UNCERTAINTIES

Perturb nominal effective area, and RMF, then use XSPEC to find best-fit model parameters for synthetic Chandra ACIS observation computed using the nominal instrument response. Compare with parameters found from fits to 1000 synthetic spectra differing only by Poisson noise and generated using the nominal area and RMF (Figs. 5 and 6). Blackbody, typically fits thermal plasma, and power law continuum models investigated. Repeat 1000 times.

- Limiting accuracy of Chandra ACIS reached in spectra with $\sim 10^4$ counts. Beyond this, errors in best-fit parameters due to calibration uncertainties completely dominate those due to photon noise.

Figure 1: Left: Truncated normal distribution (product of a Gaussian with variance σ^2 and a unimodal step function with unit density between σ_1 and σ_2), representing the distributions of calibration uncertainties used in the perturbation functions in Monte Carlo draws. Right: Illustration of a perturbation function applied to a nominal subassembly response within a given energy range. Within each energy range, μ_{sub} , a random low-order polynomial (≤ 2) is generated that is constrained to fit within the grey shaded region defined by the uncertainties σ_{sub} and σ_{sub} , and also to join up with neighboring regions within the edge uncertainty σ_{edge} . The distribution from unity for a large sample of vectors corresponds to $P(\sigma)$.

Figure 2: Left: Illustration of the relative change in the HRMA effective area caused by different hydrocarbon contamination layers. The range shown corresponds to the nominal adopted 22 ± 6 Å layer thickness. Middle: Relative change in the model ACIS S3 QE caused by $\pm 20\%$ differences in the model CCD depletion depth from that of 2.15 μ m adopted here, which corresponds to a range of about $\pm 3\%$ in the QE at 10 keV. Right: QE change caused by the adopted $\pm 20\%$ difference in CCD SiO₂ thickness.

Figure 3: True HRMA effective areas that represent the some of the uncertainties in its calibration. These models were sampled at random as part of the Monte Carlo process, with relative discrete probabilities of 1 for model F (current CALDB model) 0.5 for models A-E and G, and 0.25 for model V.

Figure 4: The nominal "best" Chandra ACIS-S effective area (black line) with a sample of 20 effective areas generated using the Monte Carlo randomization method described in the text (grey).

Figure 5: Statistical (black) vs Systematic (red) uncertainties. Example histograms (distributions of best-fit parameters obtained for typical blackbody, thermal plasma, and power law models from XSPEC) for synthetic data sets containing 10⁴ (upper panels) and 10⁵ (lower panels). Black histograms are distributions resulting from 1000 Monte Carlo realizations of the synthetic data using Plasma noise variations alone. Red histograms are the distributions of parameters resulting from fits to a single synthetic data set using 1000 Monte Carlo-generated effective areas and response matrices.

Figure 6: Statistical (black) and Systematic (red) uncertainties compared. Uncertainty on the best-fit blackbody temperature, thermal plasma temperature and power law slope as a function of total simulated count rate. Systematic errors begin to exceed statistical errors for count rates with $\sim 10,000$ counts and more. The limiting accuracy of Chandra is reached with 2,000-10,000 counts; increasing an exposure to obtain more than 10,000 counts does not increase the accuracy of the experiment.

Figure 7: Absorbed Blackbody, $N_H = 0.1 \times 10^{22}$, $kT = 0.5$ keV. Absorbed Plasma, $N_H = 0.01 \times 10^{22}$, $kT = 1$ keV. Absorbed Powerlaw, $N_H = 0.1 \times 10^{22}$, $\alpha = 1.5$.

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HRMA On-Axis: Combination of perturbation functions, $\mu_{\text{off}}(E)$, and ray-trace derived effective areas sampling the effects of differently located contamination layers and interpretations of XRCF measurements (Figs. 2.3.4).

HRMA Vignetting Function: For off-axis angle θ (in arcmin), include fractional uncertainty of vignetting function, $V(\theta)$, and Debye-Waller related function.

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$$\mu_{\text{OBF}}(E) = e^{-\mu_{\text{OBF}}(E) - \mu_{\text{OBF}}(E) + \mu_{\text{OBF}}(E)}$$

where σ_{C} , σ_{F} , and σ_{Pl} are the fractional uncertainties in the optical depths C, O, F and Fluorium at a fiducial date (2003.29).

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Monte Carlo is a nice place in the summer but we don't go there

Bugger! only in the computer do we play uncertainty games

Changing areas at random, rmfs too to estimate how

Good are slopes, kT's... we will release our code soon but not yet, bugger.