NICER CALIBRATION: Energy Scale Developments and Releases

C. B. Markwardt

Version 1.0 2019-08-08
Version 2.0 2020-07-17 - updates for optmv7 - optmv11
Version 2.1 2020-07-28 - fix glaring errors in version history (v004 - v006)

Summary and Release History

This document briefly describes improvements to the NICER energy scale since mid 2018. Based on the current release, the NICER calibration team estimates that the energy scale has the following properties:

- Nominal energies are assigned to photons in the ~0.25–15 keV band
- Estimated energy scale errors are approximately 5 eV (within 0–10 keV) and 30 eV in the 10–15 keV band

Public Release	NICER CALDB Ver	Internal Name	GCALFILE String	Comments
2018-02-26	xti20180226	rational2	20170601v001	Initial release; low quality
2018-11-05	xti20181105	optmv7	20170601v002	Energy scale known to ~5 eV over 0.25 keV–8 keV range
2019-05-16	xti20190516	optmv7h	20170601v003	Typical change above 10 keV of 10s of eV (300 eV max)
2020-02-02	xti20200202	optmv7he	20170601v004	Changes above 8 keV of ~100s of eV (1500 eV max at ~15 keV) *("August 2019 Cal Summit")*
2020-07-22	xti20200722	optmv10	20170601v005 *20170601v003_optmv10*	Typical changes of ~5 eV in 1.5-2.5 keV energy band *("March 17 2020 Release")*
2020-07-22	xti20200722	optmv11	20170601v006 *20170601v005_optmv11*	Temporal drift of zero-point reduced by 50% (~1 eV over 3 years)

Table Notes: All files appear in NICER Calibration Database as `nicer/xti/bcf/gain/nixtiflightpiSSSSSSSS.fits`, where *SSSSSSSS* is the GCALFILE String. Items listed in italics in the table are pre-release names used for internal testing purposes (not publicly released).

Introduction

The NICER energy scale, also known as its gain calibration, are key components of the NICER spectral analysis. The energy scale assigns a "true" energy to each raw pulse height. This assignment is complicated by several factors outlined below.

The energy scale calibration is often ignored by analysts, but it mustn't be. For spectral analysis, model computations are performed in "energy" space. Any error in assigning nominal energies for each event will look like a modeling error instead of an energy error. Therefore, before applying spectral response components like ARF or RMF, the energy scale must be pinned down first. Errors associated with the energy scale will be most apparent at energies where there are sharp features in the measured spectrum. For NICER, this is typically around 2.2 keV where XRC reflectivity near gold M edges has the strongest variation, but it can also occur around astrophysical edges (oxygen K, iron L, etc.). Since those energy regions are of astrophysical interest, it is the NICER team's goal to minimize energy scale errors.

We should note that when we discuss assigning an energy to each photon, we really mean assigning a **nominal** energy. The assigned energy represents an energy that would have deposited and collected 100% of the charge. However, the instrument by its nature does not collect 100% charge, or with infinite precision. There will be some resolution-related smearing as well as off-diagonal redistribution terms. The nominal energy scale is assigned so that the full photopeak centroid appears at its correct energy for known lines.

The name "optmvN" appears in many energy scale release names. The meaning of this name is

- "opt" - the energy scale model was created by "optimizing" or fitting a template gain curve to measured offsets
- "mv" - the zero-point of the system and optical loading trends are performed in detector "milliVolt" space, as opposed to pulse-height amplitude (PHA) space
- "N" - a version number
- Suffixes such as "e" or "he" indicate additional refinement, as described below.

Pulse Height (PHA) and Pulse Invariant (PI) Definitions

NICER has two collection channels, "slow" and "fast." Before calibration, pulse heights from these channels are not meaningful by themselves. Raw pulse height values are not comparable to any standard, nor between modules, nor even for the same module at different times. The uncalibrated pulse heights are identified in FITS files as

- PHA = uncalibrated raw slow-channel pulse height
- PHA_FAST = uncalibrated raw fast-channel pulse height.

After calibration is applied, the new energy scale is known as "pulse invariant" or PI. The PI values are intended to be comparable between modules and stable over time. The calibrated column names are PI and PI_FAST.

- PI = calibrated slow-channel pulse height
- PI_FAST = calibrated fast-channel pulse height.

The definition of PI is:

1 PI unit = 10 eV.

PI values refer to the bottom edge of the bin. Thus, a PI value of 600 refers to a bin that covers the nominal energy range 6.00–6.01 keV, and is centered at 6.005 keV.

For the most part, the "fast" channel is not used for spectral analysis, and has not been a strong focus of NICER calibration efforts. Calibration releases are intended to maximize performance of the slow channel ("PI").

Additional NICER Energy Scale Challenges

NICER performed extensive energy-scale calibrations before launch. Unfortunately, these calibration products were not easily useful after launch. With several post-launch years of experience we now know of multiple challenges that have made deriving an energy scale more difficult and time consuming.

NICER's energy scale shifted. Before launch, or early after launch, the NICER energy scale shifted compared to the time of the pre-launch calibration measurements. The cause of this shift, and the exact nature of the shift, are unknown. Thus, we have been required to reconstruct a best-effort energy scale using calibration references accessible on-orbit. This has been an iterative procedure, resulting in incrementally improved energy-scale releases.

NICER's energy scale depends on the amount of optical light. NICER's detectors are sensitive to both X-ray and optical light. A certain amount of optical blocking is achieved using

window filters, but some light does pass through these filters. Optical light loading contributes both an offset to the energy scale (zero-point shift), as well as an increase in noise electrons.

NICER's energy scale is temperature-dependent. For the most part temperature-related effects were known pre-launch and have been assumed to remain correct. Since NICER's environment on the International Space Station is quite temperature-stable (~30–45 C), this has not been a significant issue.

Calibration Procedures to Develop the optmv7 Energy Scale Model

As noted above, NICER experienced post-launch shifts in its energy scale. NICER has no on-board dedicated energy calibration device (i.e., no Fe55 radioactive source). Therefore, the NICER team has for the most part used astrophysical reference targets for its energy scale calibration.

For energy scale zero-point, most changes are driven by optical loading. NICER's on-board system takes samples of both input channels at a 5 Hz rate. These are known as "forced triggers," but are essentially triggerless measurements of the input noise level in both channels. Although forced trigger data are available for every observation, it is not possible to measure an accurate centroid of the zero-point unless thousands of seconds of time are averaged. Since lighting conditions on the ISS change more rapidly than that time scale, we use an alternate approach.

The so-called "undershoot" reset events are a proxy indicator for optical loading. We use a mission-long database of forced trigger event data and correlate with undershoot rate. Figure 1 shows a sample of variations of the zero-point, expressed in milliVolts, with undershoot rate.
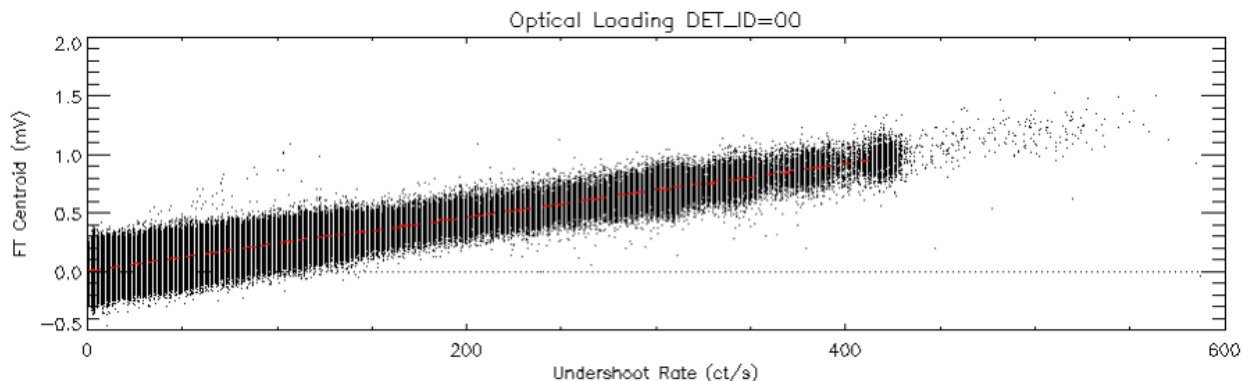
Figure 1. Variation of forced trigger centroid position (zero-point shift) with undershoot rate (optical loading) for detector 00 for the time range 2017-07-01 to 2018-01-30. Each point represents the average of 1 second of forced trigger values. The red line is a linear trend.

Evidently, the variation of zero-point is quite linear with undershoot rate, and is reproducible. We estimate these trends for each detector. Using this knowledge, we can use the per-detector undershoot rate available at any time to determine the amount of zero-point shift due to optical loading.

For the overall gain scale, we require a set of known and stable reference energies that can be accurately measured by a non-imaging instrument such as NICER. Here are the reference energies we have used for NICER calibration:

- Vela X-1 line at 6.4 keV. This line is isolated and sharp according to Chandra grating observations. It can be measured to within ~10 eV by each detector module. This feature is heavily weighted.
- 1E 0102 supernova remnant, line complexes of Oxygen and Neon below 1 keV. These lines are not well resolved by NICER, but the relative norms and energies are well-known based on grating observations by Chandra and XMM, again to about 10 eV.
- Gold M edge at ~2.2 keV seen in Crab observations. This edge is not sharp but it is very strong against the continuum emission of the Crab nebula.
- Oxygen K edge at ~535 eV seen in Crab observations. This edge has significant fine structure which has been measured by XMM gratings, which we include in the model.

We also considered other features but rejected them, or included them with only light weighting.

- Strong Al and Si fluorescence lines appear during SAA passages. However, it is likely these lines are strongly broadened and shifted by the so-called ballistic deficit effect due to far off-center X-rays. These features were deemed unreliable and excluded.
- Strong Au L-shell and Ni K-shell fluorescence lines appear during SAA passages in the 7–14 keV range. The origin of these lines is not completely clear and may be due to fluorescence from either the XRCs which have gold reflective surfaces, the "traffic cone" radiation shields which are plated with gold, or from gold inside the FPM packaging (such as gold bond wires). Because of this uncertainty, these lines were included but at much lower weight.

For these reference lines, spectra were extracted from the data on a per-detector basis, and fitted with the nominal response matrix. We used the XSPEC "gain fit" capability to perform minor adjustments to the energy scale. The result was a set of energy offsets for each detector at the above-mentioned lines or edge features.

Figure 2 shows two example spectra for the Au M and O K edge structures for observations of the Crab nebula.
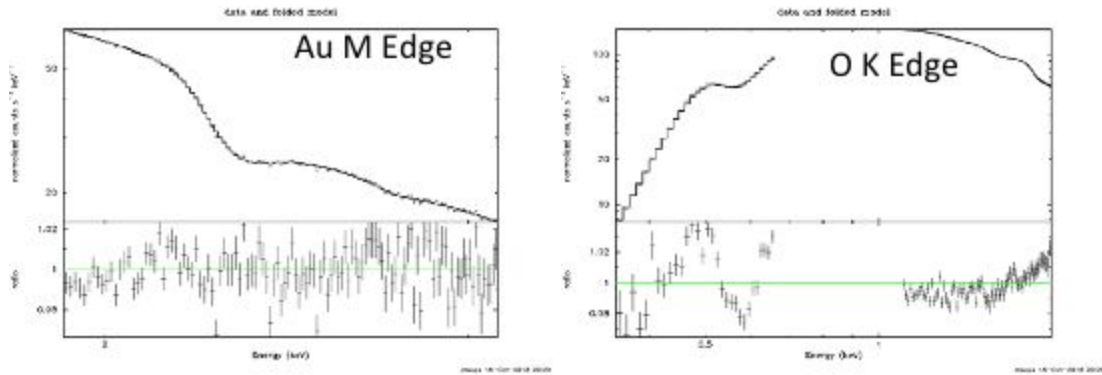
Figure 2. NICER array-average spectrum in the Gold M (~2.2 keV) and Oxygen K (~0.54 keV) ranges. The gain scale was adjusted to provide the best fit on a detector-by-detector basis.

Figure 3 shows a sample spectrum of Vela X-1 in the Fe K range. It demonstrates that a centroid can be accurately measured (~10 eV uncertainties). We also attempted to measure temperature-related variations of the energy scale by dividing the data into low and high temperature data, using the median MPU temperature of 36.5 C as a dividing point. No significant variations with temperature were detected.
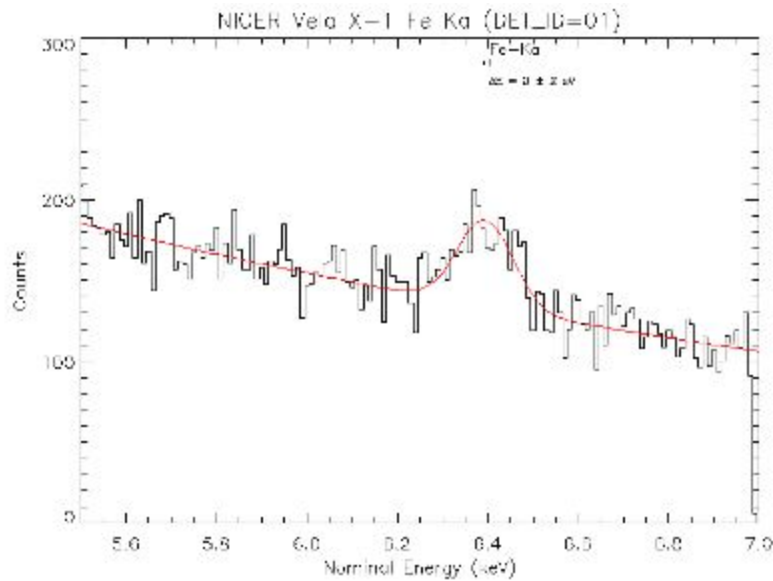

Figure 3. Spectrum of Vela X-1 in the Fe K (~6.4 keV) range for detector 01. The best-fit model contains a power-law continuum and sharp line at the Fe Ka energy. Broadening here is due to the detector response model.

After this process was complete, we had obtained energy offsets for each detector. We then adjusted the gain curve of each detector based on these data points.

Figure 4 shows a sample of such offsets for a particular NICER detector. All offsets are measured relative to the pre-launch calibration system. The chart demonstrates that significant

offsets are present in the NICER energy scale, as large as 100 eV at the top of the energy range. The two curves are attempts to smoothly interpolate these offsets.
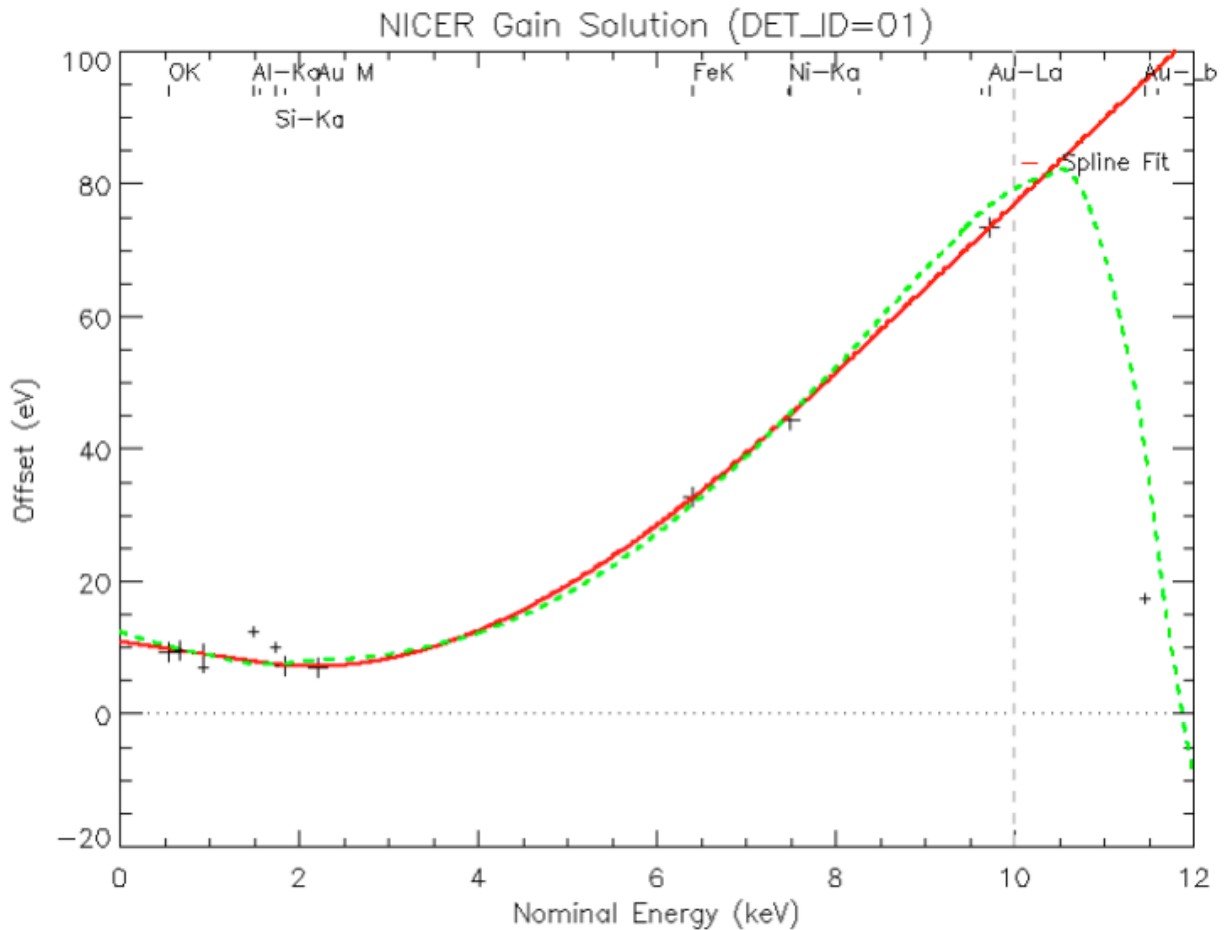

Figure 4. NICER measured energy offsets for detector 01 as a function of energy. The lines are labeled by their features at the top of the plot. The red curve is a spline fit to data below 10 keV; the green curve is a more appropriate fit using the detector's gain curve itself as a fitting template.

The plot demonstrates that at low energies, the typical post-launch offsets are around 10 eV, but increase to higher energies, with a maximum shift of ~100 eV.

After obtaining a smooth correction curve, the residuals are shown in Figure 5. Generally speaking, the fits are quite excellent, although the behavior at high energies, above 10 keV, was less well understood at this point and was refined in later releases.

This result of this effort was the "optmv7" calibration release. This was a major change to NICER's energy scale calibration and represented a large step forward. After this point, further changes have been incremental and typically small in NICER's primary bandpass below 10 keV.
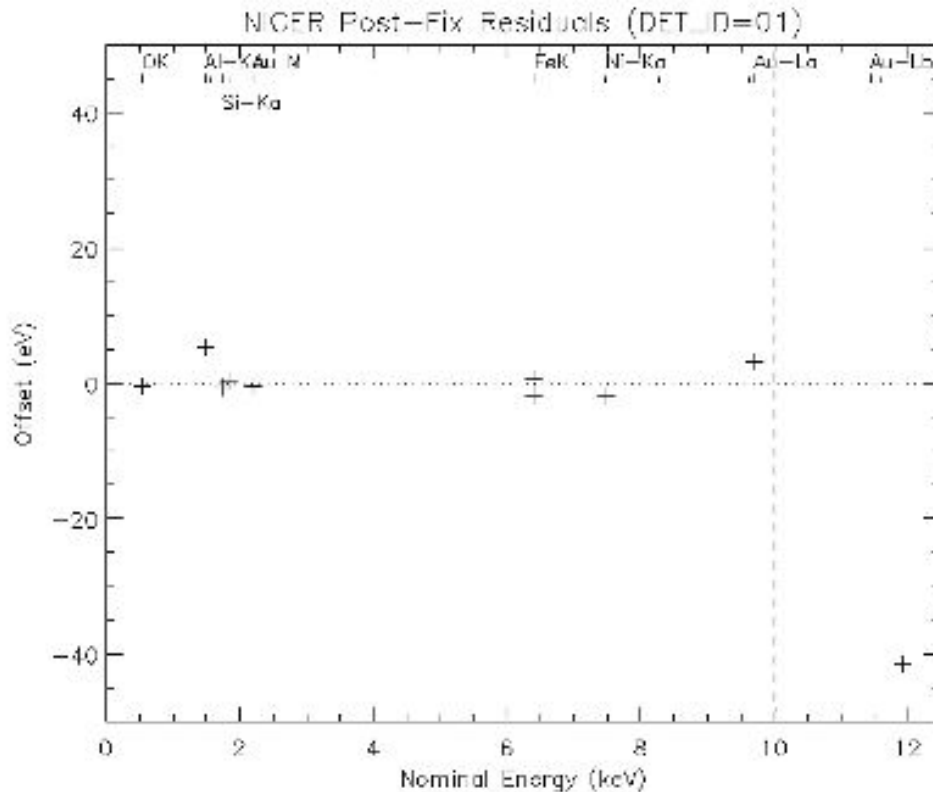
**Figure 5.** Post-fit residuals after applying the spline calibration of Figure 4.

After completion, "optmv7" resulted in significant improvements to the energy scale. We now discuss additional developments after optmv7.

optmv7e Energy Scale Model Development

The NICER optmv7e model (released publicly May 2019 as gain file nixtiflightpi20170601v002.fits) contains improvements to the NICER energy scale primarily above 12 keV. Calibration work revealed that the pulse height to charge conversion table had irregularities above a certain energy, typically above 12 keV. These irregularities could manifest themselves as certain pathological conditions, such as non-monotonic energy scale (i.e., energy scale "going backwards") as well as discontinuous jumps. These effects were the result of edge effects introduced during the 2018 grand calibration effort. Here "edge effects" means the effect of interpolation interference at the upper boundary of the table around 15–18 keV. The solution was to perform a smooth fit to the data below the discontinuities and extend that fit to higher energies.

Figure 6 shows an example of the approximate energy to channel relation for DET_ID 50. After correction, the artifact above PHA 3900 is removed.
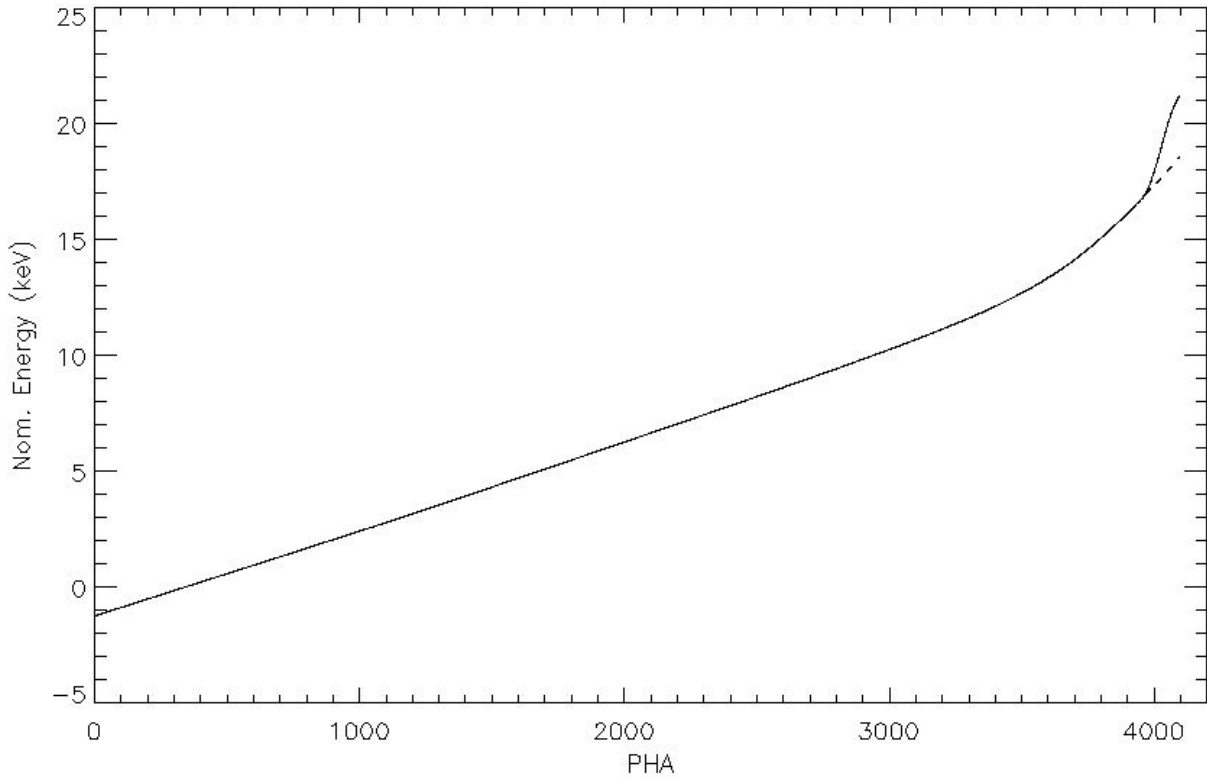
F**igure 6.** Approximate energy to channel relation for NICER DET_ID 50. The optmv7 (old) solution is solid; the optmv7e (new) solution is dashed.

Figure 7 shows the difference between the optmv7 baseline and the optmv7e improvement for all NICER modules stacked together.
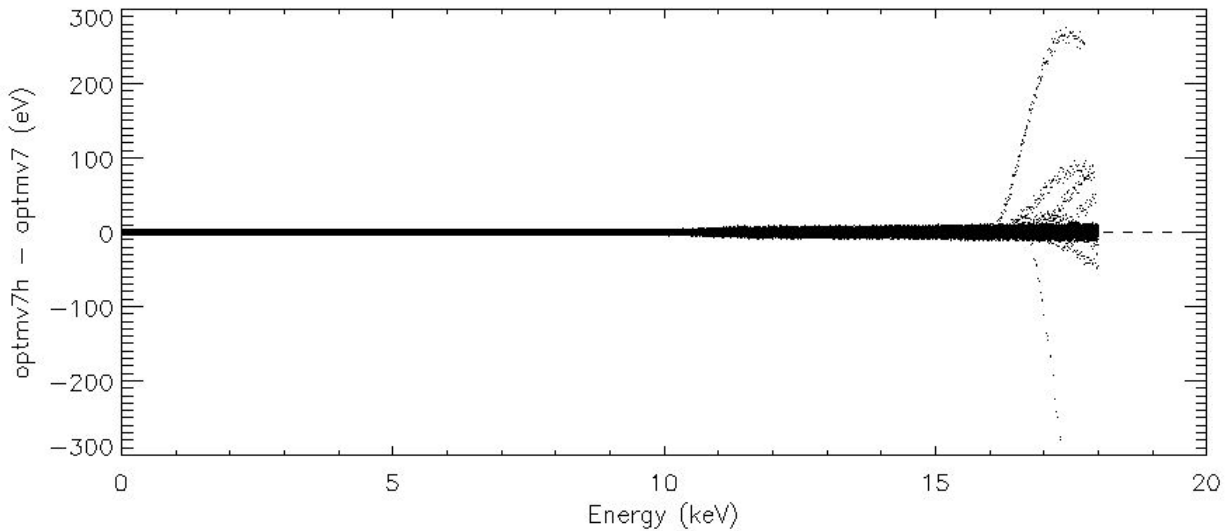
F**igure 7**. Difference between optmv7e and optmv7 over the entire NICER energy range.

The plot shows that almost all of the change is above 15 keV, although there are small changes at the 10–20 eV level in the 10–15 keV range. There is no change below 10 keV.

optmv7he Energy Scale Model Development

The next energy scale development, dubbed optmv7he, further improves the energy scale at the high energy range above 10 keV.

During the grand calibration work of optmv7, we made several assumptions about how the energy scale would behave at low energies and extrapolated this trend to high energies.

The NICER slow-channel energy scale contains a "kink," typically at about 10 keV, where the energy to channel relation changes slope.   The fast channel does not have any kink, or at least it is much reduced. In Figure 1, above the change in slope is gradual and occurs at about PHA 3500, but each detector is unique. In some detectors the "kink" is sharper. During the grand reprocessing, we had little information about how the "kink" would behave after the post-launch shifts.

For optmv7he, we used the fast channel as a reference baseline. We used a dataset composed of all background fields, which contains both high and low background levels, but importantly it contains background events that span the full NICER energy range. In some sense this is a "flat field" that fills the energy range with a nearly uniform set of events. Figure 8 shows an example of this trend as a density histogram.
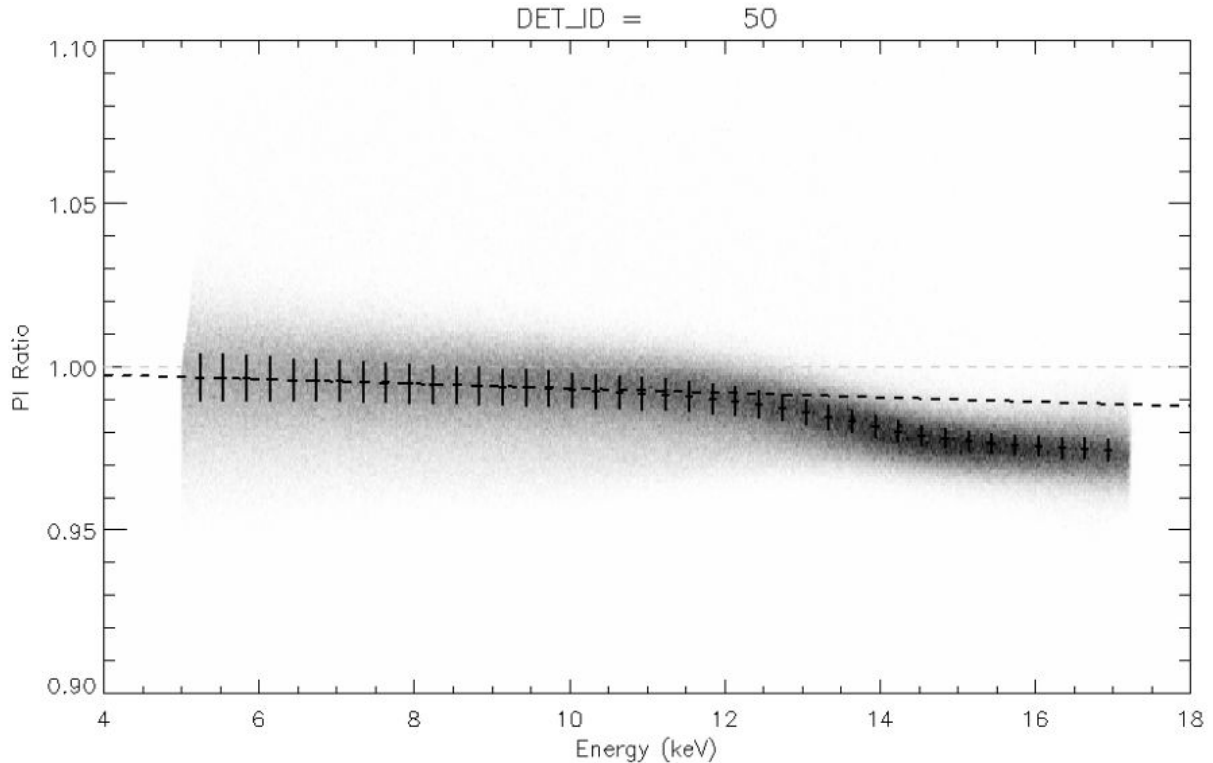
Figure 8. 2D density histogram of PI_RATIO (vertical) and energy (horizontal; slow channel) for NICER background events in DET_ID 50. The "expected" unity line is shown as a light gray dashed line. Also shown are the centroids of the density histogram slices in 300 eV steps (crosses); and the linear fit to the crosses in the 5.5–8 keV band (dashed line).

We measured the PI ratio (PI / PI_FAST) of all those events at each energy slice (in the narrow ratio range of 0.9–1.1). Here the slices were 300 eV. Nominally all events should lie on the flat ratio of 1.0. Any deviations can reflect an error in the energy scale of the slow or fast channels.

Assumptions made:

- The fast channel does not have significant sharp variations of energy to channel, so any such variations seen are errors in the slow channel (fast channel errors are at worst linear with energy)
- Any biases introduced by using a non-imaged background are negligible (the centroid of the background represents the centroid of an imaged source).

We do allow for errors in the fast channel. We fit the ratio offsets in the 5.5–8.0 keV range with a linear trend. In this energy range the slow channel error should be effectively zero because we had effective energy calibration lines to measure in the slow channel. Thus, any error in that range can be attributed to a fast channel error. We extrapolate that trend to higher energies. Any deviation of the ratio from this trend line above 8 keV, we attribute as a slow channel error.

The question of biases introduced by a non-imaged background are interesting to consider. In principle, a non-imaged source of counts such as background, which interacts at all detector positions, will have a different PI_RATIO than an imaged source, which interacts at the center. This is because the electron charge cloud spreads out due to diffusion as it travels inward to the collection point. Charge clouds from interactions farther from the detector center travel farther, and thus diffuse more, which can change the rise time. This is known as the "ballistic deficit" problem.

However, in practice the mean ballistic deficit is small, typically 10s of eV, and is likely to be negligible. Furthermore, it varies approximately linearly with energy. Since we fit out a linear error trend, most of the non-imaged biases will be removed. Finally, above 8 keV, we simply do not have many well established references that can be used for calibration purposes. This technique is the best we can do. Unlike the performance below ~8 keV, where we typically promise ~5 eV energy scale errors, above 8 keV, we will likely have to admit higher errors, typically ~50 eV.

The final corrected slow-channel energy is computed as:

NEW_SLOW = OLD_SLOW x (Extrapolated trend) / (PI_RATIO centroid)

where "Extrapolated trend" is the linear trend extrapolated to all energies; and "PI_RATIO offset" is the centroid measured in the plot above. The adjustment was only done above 8 keV; below 8 keV no change was made. This new correction ("optmv7he") was captured for each module and embedded in a new pulse height conversion table.

Figure 9 shows the performance of optmv7he compared to the baseline of optmv7, as a function of energy.
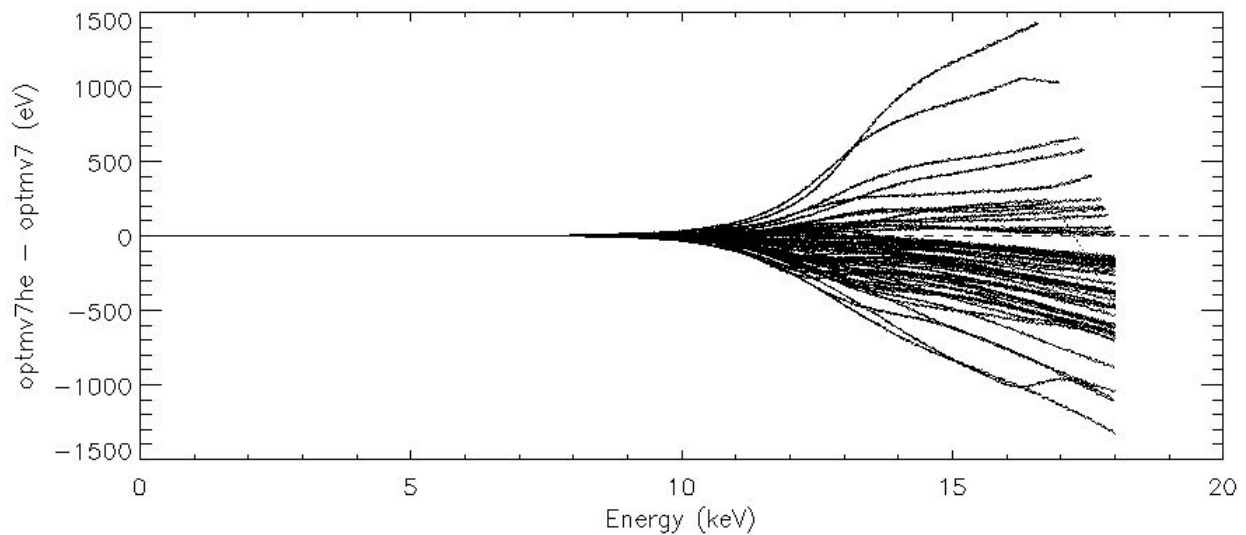
Figure 9. Difference between optmv7he and optmv7 over the entire NICER energy range.

This figure has a different vertical scale than Figure 2 because the adjustments are much larger. The mean change above 8 keV is –62 eV while the standard deviation is 220 eV. Above 12 keV the changes are larger still: mean change of –138 eV and a standard deviation of 328 eV. The maximum change is about 1500 eV.

Note that in the figure above the top traces stop before they reach 18 keV. This is because for these detectors the maximum digitized pulse height value of 4096 occurs below 18 keV.

optmv7he Performance: SAA Lines 8–14 keV

After adjusting the energy scale based on optmv7he, we examined data from NICER's SAA passages. These data contain fluorescent lines of Nickel and Gold near the instrument, stimulated by passages through charged-particle zones. These lines should occur at precisely known energies. Before the application of this procedure, most of the lines above 10 keV were washed out and not detectable. After application they are detectable and sharp. Table 1 shows the expected transitions for nickel and gold for proton bombardment.

Atom	Transition	Energy [keV]	Approx Intensity [arbitrary]
Ni	$K\alpha1/K\alpha2$	7.477/7.460	66.313+33.687
	$K\beta1/K\beta3$	8.263	8.442+4.304
Au	Ll	8.493	5.050
	$L\alpha1$	9.712	89.788
	$L\alpha2$	9.626	10.212
	$L\eta$	10.307	0.8284
	$L\beta1$	11.440	30.135
	$L\beta2$	11.583	19.735
	$L\beta3$	11.608	2.576
	$L\beta4$	11.203	2.226
	$L\beta5$	11.914	2.1935
	$L\beta6$	11.158	1.2489
	$L\gamma1$	13.379	6.298

	Lγ2	13.707	0.5781
	Lγ3	13.807	0.727
	Lγ4	14.297	0.2341
	Lγ5	12.972	0.2131
	Lγ6	13.728	0.6272

Table 1. Expected line transitions from proton bombardment of Au and Ni. Transitions are given in Siegbahn notation. Line centers and approximate intensities from Crawford et al. 2011 (ANSTO/E-774). Intensity units are arbitrary and can only be compared relatively within the same atom and major transition, and are set so that the intensity sum $\alpha1+\alpha2 = 1$.

Line intensities come from theoretical estimates of bombardment of these atoms by 3 MeV protons (Crawford et al. 2011, "Calculated K, L and M-shell X-ray line intensities for light ion impact on selected targets from Z=6 to 100," ANSTO/E-774), and are only approximate indications for NICER's actual SAA conditions.

Figure 10 shows the SAA spectrum, summed from July 2017 through July 2019. The plot shows that all lines of gold up to the ~13.4 keV Lγ complex are recovered.
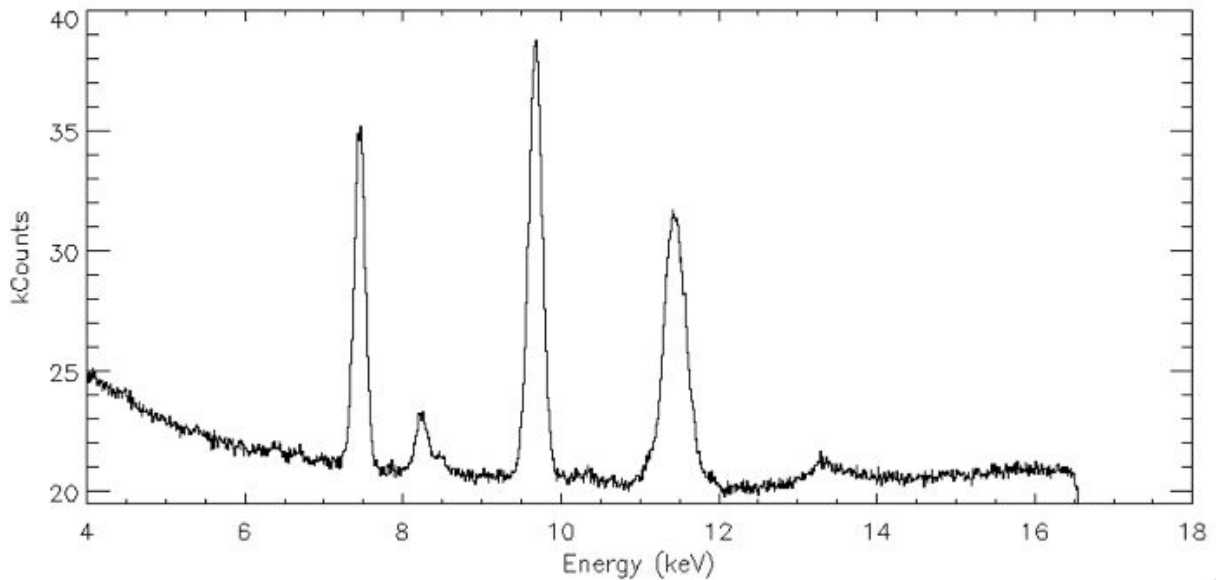

Figure 10. Full-array spectrum of NICER data when passing through SAA. Fluorescent Ni K and Au L lines are visible as described in the text and Table 1.

optmv10 Developments

The next development, named "optmv10," reflects an iterative improvement over previous gain models. When studying the results of the optmv7he model, it was found that there were sharp "kinks" in the calibration curves for most modules between 1.5 and 2.5 keV. There are no physical reasons to expect sharp features in the detector calibration curves. We suspect that pre-launch calibration measurements of these curves introduced these features. The pulse injection equipment used for pre-launch measurements has a range shift in approximately this energy band.

Figure 11 shows an example of the effect, for detector ID 01. The black curve is the calibration curve of optmv7he, before adjustment. We adjusted each curve on a detector-by-detector basis. We created a cubic interpolation curve based on the 3-4.5 keV range and extrapolated it to lower energies. We also used energy offsets measured from Crab data of the O K, Si K, and Au M to inform the creation of the new spline curve, although Si K suffers strong systematics and is weighted only very weakly. The results are new, smooth calibration curves for each detector.
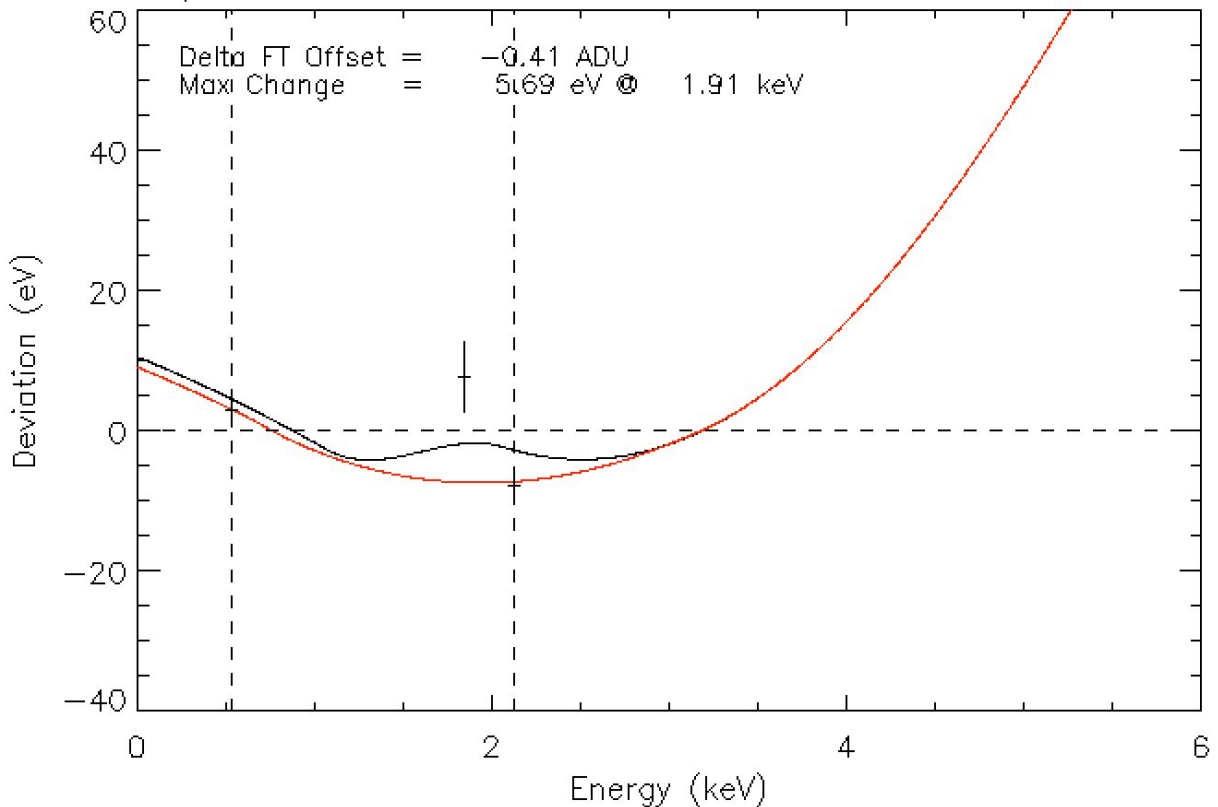
Figure 11. Example calibration curve of NICER detector 01 in the 0–6 keV range. Curves are shown as deviations from a linear trend expressed in eV. Pre-adjustment (black) and post-adjustment curves are shown. Measured offsets of the O K (0.533 keV), Si K (1.840 keV) and Au M (2.210 keV) edges taken from Crab observations are shown as points. The maximum change after adjustment for this detector is 5.69 eV at 1.91 keV.

The largest change is in the 1.5–2.5 keV band, with a typical adjustment magnitude of 5 eV, although curve values between 0–3 keV were adjusted to some degree for every detector by a few eV. Bear in mind that one NICER PI bin is 10 eV, so most of these changes are at the fractional pulse height bin level. Analysis of the Crab data shows changes in residuals of less than 1% after applying this adjustment.

optmv11 Developments

After nearly three years in operations, we took time to examine the long-term behavior of NICER's gain calibration.

The first step was to look for drift of NICER's zero-point. This is routinely measured using the forced trigger system as mentioned above, so there are large amounts of data to be analyzed. The nominal "energy" of forced triggers should be 0 keV. Any deviation from 0 would indicate a calibration shift. Note that since forced trigger measurements are statistical in nature, it is possible for individual values and mean values to appear negative after calibration. This of

course does not mean that energy is negative. This can occur statistically, say fluctuations both below (and above) 0 keV; but it can also occur if there are systematic trends in the data. Thus, we plot the systematic forced trigger zero-point for every detector.

A linear trend term was added to the energy calibration term after launch, and reflects the trends measured in the first six months. However, we now have additional data which can be used to verify these trends.

Figure 12 shows such a trend plot on a detector-by-detector basis. It is clear from this plot that there are indeed zero-point drifts that increase with time. Some zero-points increase and some decrease with time. The average value is 0.33 eV/yr, with standard deviation of 1.07 eV/yr.
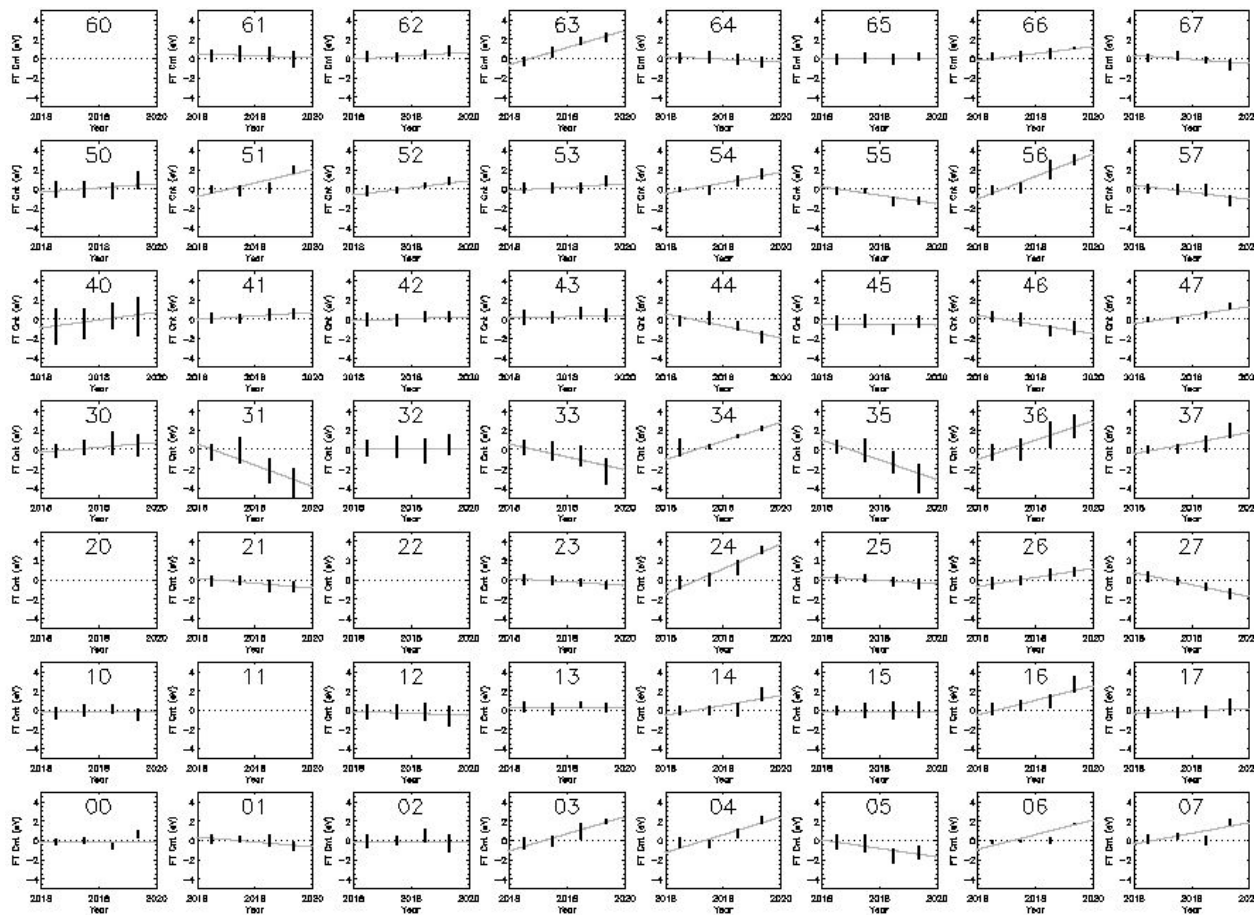
Figure 12. NICER forced trigger zero-point trending for all 56 detector modules, covering the range July 2017–July 2019. Each point is an average of 6 months with statistical error bars. A linear trend is shown to guide the eye. The Y axis is labeled in eV with a range from –5 to +5 eV.

Based on data through mid-2020, it appears that the zero-point linear drift measured six months after launch was correct, but since that time, the drift rate has decreased. Thus, the post-launch drift correction has overcompensated the true drift rate. The typical overcompensation is about a factor of 2x, i.e., the correct long-term value is about 50% of the post-launch value. We have

adjusted these trend values. Since the adjustment is of order 0.33 eV/yr, over a 3-year mission the average change is about 1 eV or only 10% of a 10 eV pulse height bin. After applying this change, the Crab spectrum changed negligibly (<0.1%).

Summary of Energy Scale Performance

In summary the NICER energy scale is known to about 5 eV in the 0–10 keV band, and to about 30 eV in the 10-15 keV band.

Figure 13 shows energy centroid residuals as measured for astrophysical targets observed by NICER, as a function of energy. These represent deviations of NICER estimates compared to "best-known" or canonical reference energy values. This plot generally represents our claim that the NICER energy scale is known to about 5 eV over its primary science band. However, it should be interpreted with some caution as well. In some cases, we may be testing the limit of astrophysics: the deviations could reflect real deviations (red/blue doppler shifts) from canonical values. This may be true for expanding supernova remnant shells, as well as X-ray binaries, which may have orbital doppler shifts or broadening. Despite these caveats, this real data indicates that NICER's energy scale performance is excellent.
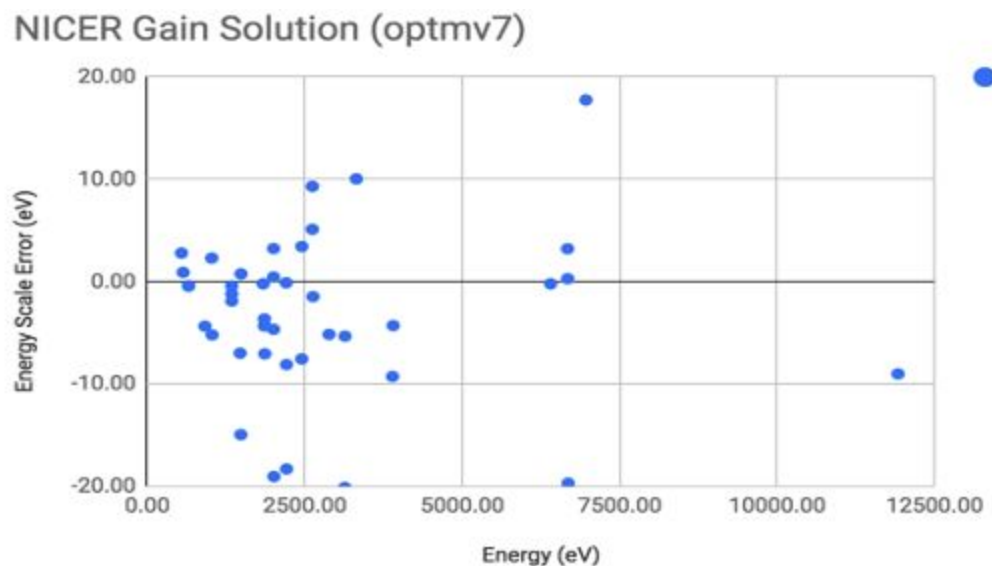
Figure 13. Residual energy shifts for astrophysical targets in the NICER energy band as of early 2018. Included are observations of GX 301–2, Perseus Cluster, WR 140, Eta Car, Cas A, HR 1099, Coma Cluster, 1E 0102, N132D, Cen X-3, Vela X-1, SAA, UX Ari, and GT Mus.

Caveats For Recalibration

For the general user there are a few caveats to bear in mind when using the new NICER energy scales.

It is recommended to use 'nicerl2' to completely reprocess your data from scratch.

However, it is possible to run 'nicerpi' with recal=YES, and recalibrate an existing cleaned and screened event file. There is a "gotcha" with this technique, however. When you do this, the original unscreened event file is not available: the event energies are adjusted in place. **The gotcha occurs at the edges of the energy boundary used for selection.** Say for example that photons with event energies 0.5–3.0 keV were selected. After recalibration, some photons will be moved upward or downward. A sample photon at 2.99 keV might be moved to 3.01 keV, out of the energy range of interest but it is still listed in the event file.

Even worse, if the user had worked with the unscreened event file, there would also be photons at 3.01 keV in the original unscreened event file that would potentially have moved down to 2.99 keV, but if you work with only the screened event list, this photon is not available to move down, and this creates an artificial deficit just below the upper energy boundary. Thus, there will be subtle edge effects around the boundaries of energy selection. As long as the user selects a wider energy range than the true range of interest, and then only downselects when performing the final analysis, recal=YES is a useful option. The amount of extra margin should be comparable to the change in gain solution noted above.

Also, for purposes of comparison, you may wish to run an old versus new comparison. Please be aware that 'nicerpi' uses a randomizer at the sub-PHA level. This will lead to **off-by-one differences between the old and new event lists** which are entirely expected.