Chandra X-ray Center

Memo: Generalize the temperature dependence of CTI in CALDB CTI files and acis_process_events

Revision 1.0—09 Mar 2023

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Document and Change Control Log			
Date	**Version**	**Section**	**Status**
09 Mar 2023	1.0.0	all	Initial version

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1 Summary

In the future, ACIS will have to be operated over a wider temperature range than it currently is. CTI is highly temperature dependent and the current parameterization is unable to describe this to sufficient accuracy.

This memo presents a scheme to accommodate this with minimal changes to existing CALDB formats and the existing `acis_process_events` implementation. It sets out background and motivation and a spec for the **changes** that are required; it does not replace existing ICDs and specs; instead, the changes described will have to be incorporated into those existing documents.

The changes involve three additional columns in the CTI file, and an additional, third, image dimension to the CTI_IMAGE files, together with I/O changes to `acis_process_events` to handle these changes and pass on the relevant data subset to the existing, unchanged, algorithm.

2 Motivation

The Chandra X-ray Observatory (CXO) is aging, and thermal management is becoming a more and more difficult task for mission operations. Observations longer than 20 or 30 ks are already rare, and, without raising the allowed temperature for the ACIS focal plane, observations will have to become even shorter. This places severe constraints on mission planning, but also limits certain science cases that would benefit from longer uninterrupted observations. Observations with the gratings are already allowed to be executed at higher temperatures than ever before, but the vast majority of observations with Chandra are done with ACIS for imaging. Thus, changing the allowed temperature range for ACIS imaging observations would have a much bigger positive impact on mission planning; it might in fact be required in the future to do any observations at all in certain regions of the sky.

There is one major hurdle: CTI is strongly temperature dependent. CTI effects come into play in at least two areas of data processing: First, CTI moves the centroids of the distribution of PHA values observed for any given energy and this effect is corrected for in `acis_process_events`; second, CTI broadens the distributions, which is represented in the RMF, and thus needs to be taken into account in `mkacisrmf`.

The first effect is more severe from an analysis standpoint, because it leads to a systematic offset in energy, while a little broadening of the RMF in ACIS data that's already low-resolution has less of an effect in many scenarios. Also, `acis_process_events` is run in pipeline processing and thus needs to be addressed for both DS and CIAO releases. *This memo only addresses changes to `acis_process_events` and related CALDB files; any changes to `mkacisrmf` are developed separately.*

2.1 The need to generalize the existing mechanism for CTI temperature dependence in `acis_process_events`

`acis_process_events` already includes a temperature dependence of the CTI encoded in the `$CALDB/data/chandra/acis/cti/*` files (see 4). These files contain coefficients to describe a temperature dependence for some parts of the mathematical equation used to correct for CTI (these equations are given Ref. 3 and implemented in `acis_process_events` in the current version CIAO 4.15). However, this scheme was designed to work for a relatively narrow range of temperatures. Initial calibration observations at higher temperatures show that this is insufficient to describe the behavior of CTI over the wider range of temperature currently forseen by mission planning and the calibration group (see presentations to the ACIS calibration group in Jan, Feb, and March of 2023).

2.2 Urgency

The decaying thermal performance makes scheduling observations more and more difficult already; on the other hand, we cannot deliver data to observers that cannot be reduced and analyzed with the available DS and CIAO versions. Thus, observations at higher temperatures should not be done before the required changes are implemented in the DS pipeline and CIAO. According to mission planning, this needs becomes more and more pressing and we may out significant constraints on scheduling flexibility, if we delay this to the DS or CIAO releases in mid- and late 2024.

3 Scope

3.1 Scope of applicability

This interface shall apply to all ACIS observations as processed by the tool `acis_process_events` and distributed to the CXC Data Archive during the course of the Chandra mission.

3.2 Scope of this memo

This memo describes a small and specific change to `acis_process_events` (see 1 for the `acis_process_events` spec and refs 2 and 3 for the CTI equations in particular). The `acis_process_events` spec (Ref. 1) is a massive collection of formulas, which makes it hard to understand the intent of individual changes, which is why we describe it here in a separate memo. The CTI formula in `acis_process_events` is described in Ref. 2, last updated in Ref. 3. That formula remains unchanged, what changes is how the coefficients used in that formula are loaded from the CTI files in the CALDB.

4 Applicable Documents

The Applicable Documents required for background and detail are as follows:

1. `acis_process_events` spec:
   `https://space.mit.edu/cxc/docs/ape_spec_4.17.pdf`
2. memo: Adjusting ACIS Event Data to Compensate for the CTI; version 7.2 `https://space.mit.edu/CXC/docs/docs.html#cti`
3. memo: Adjusting ACIS Event Data to Compensate for the CTI; version 7.3 (distributed by email by D. Principe in 2018)
4. AXAF CALDB Architecture
   `https://cxc.cfa.harvard.edu/caldb/index.html`

5 CALDB format and `acis_process_events` implementation

5.1 Temperature dependence in CTI in CIAO 4.15

The temperature dependence is encoded in the `$CALDB/data/chandra/acis/cti/*` files in the CALDB. These files have the following structure:

```
dmlist acisD2020-01-01ctiN0009.fits blocks

--------------------------------------------------------------------------------
Dataset: acisD2020-01-01ctiN0009.fits
--------------------------------------------------------------------------------

     Block Name                          Type         Dimensions
--------------------------------------------------------------------------------
Block    1: PRIMARY                        Null
Block    2: AXAF_CTI1                      Table        21 cols x 10       rows
Block    3: AXAF_PCTI_IMAGE0               Image      Real4(1024x1024)
Block    4: AXAF_PCTI_IMAGE1               Image      Real4(1024x1024)
```

```
Block    5: AXAF_PCTI_IMAGE2              Image      Real4(1024x1024)
Block    6: AXAF_PCTI_IMAGE3              Image      Real4(1024x1024)
Block    7: AXAF_PCTI_IMAGE4              Image      Real4(1024x1024)
Block    8: AXAF_SCTI_IMAGE0              Image      Real4(1024x1024)
Block    9: AXAF_PCTI_IMAGE5              Image      Real4(1024x1024)
Block   10: AXAF_PCTI_IMAGE6              Image      Real4(1024x1024)
Block   11: AXAF_SCTI_IMAGE1              Image      Real4(1024x1024)
Block   12: AXAF_PCTI_IMAGE7              Image      Real4(1024x1024)
Block   13: AXAF_PCTI_IMAGE8              Image      Real4(1024x1024)
Block   14: AXAF_PCTI_IMAGE9              Image      Real4(1024x1024)
```

The first relevant block is the table in block 2 which has the following columns:

```
dmlist acisD2020-01-01ctiN0009.fits cols

--------------------------------------------------------------------------------
Columns for Table Block AXAF_CTI1
--------------------------------------------------------------------------------

ColNo  Name                 Unit        Type             Range
   1   CCD_ID                            Int2            -                    The ID number of the CCD of a region
   2   CHIPX_LO             pixel        Int2            -                    The lower CHIPX boundary of the region
   3   CHIPX_HI             pixel        Int2            -                    The upper CHIPX boundary of the region
   4   CHIPY_LO             pixel        Int2            -                    The lower CHIPY boundary of the region
   5   CHIPY_HI             pixel        Int2            -                    The upper CHIPY boundary of the region
   6   NPOINTS                           Int2            -                    The number of PHA elements for the region
   7   PHA[46]              adu          Real4(46)       -Inf:+Inf            The PHA vector for the region
   8   VOLUME_X[46]                      Real4(46)       -Inf:+Inf            The effective charge volume for serial CTI
   9   VOLUME_Y[46]                      Real4(46)       -Inf:+Inf            The effective charge volume for parallel CTI
  10   FRCTRLX                           Real4           -Inf:+Inf            Fraction of charge trailed one pixel (serial)
  11   FRCTRLY                           Real4           -Inf:+Inf            Fraction of charge trailed one pixel (parallel)
  12   VFTRLX                            Real4           -Inf:+Inf            Fraction of charge trailed two pixels (serial)
  13   VFTRLY                            Real4           -Inf:+Inf            Fraction of charge trailed two pixels (parallel
  14   TCTIX                             Real4           -Inf:+Inf            Frac. change in serial trap density per deg C
  15   TCTIY                             Real4           -Inf:+Inf            Frac. change in parallel trap density per deg C
  16   TCTIX2                            Real4           -Inf:+Inf            Frac. change in serial trap density per deg C
  17   TCTIX3                            Real4           -Inf:+Inf            Frac. change in serial trap density per deg C
  18   TCTIX4                            Real4           -Inf:+Inf            Frac. change in serial trap density per deg C
  19   TCTIY2                            Real4           -Inf:+Inf            Frac. change in parallel trap density per deg C
  20   TCTIY3                            Real4           -Inf:+Inf            Frac. change in parallel trap density per deg C
  21   TCTIY4                            Real4           -Inf:+Inf            Frac. change in parallel trap density per deg C
```

The CTI correction formula depends on the chip, the location, the PHA value, and the AXIS focal plane temperature at the time that a particular photon is detected. That temperature changes during an observation and is taken from the Mission time-line file (see 3). The rows in the table contain coefficients for the CTI correction (see 3) and `acis_process_events` needs to select the appropriate row for each detected photon and then use the coefficients in that particular row to evaluate the CTI correction formula. Column 1-5 are used for the selection; the remaining columns hold the information for the CTI correction formula (collectively called "coefficients" for simplicity in the remainder of this text). In the CALDB distributed with CIAO 4.15, columns 1-5 look like this:

```
dmlist acisD2020-01-01ctiN0009.fits"[cols CCD_ID,CHIPX_LO,CHIPX_HI,CHIPY_LO,CHIPY_HI]" data

--------------------------------------------------------------------------------
Data for Table Block AXAF_CTI1
--------------------------------------------------------------------------------

ROW    CCD_ID     CHIPX_LO   CHIPX_HI   CHIPY_LO   CHIPY_HI

     1          0            1       1024            1       1024
```

2	1	1	1024	1	1024
3	2	1	1024	1	1024
4	3	1	1024	1	1024
5	4	1	1024	1	1024
6	5	1	1024	1	1024
7	6	1	1024	1	1024
8	7	1	1024	1	1024
9	8	1	1024	1	1024
10	9	1	1024	1	1024

So, if `acis_process_events` processes a photon detected on CCD_ID=4, at CHIP_X=345 and CHIP_Y=876 at a focal plane temperature of FP_TEMP=-119.6 C=153.55 K, then it uses the coefficients found in row 5.

The remaining blocks in the CALDB file contain the serial (not available for all CCDs) and parallel trap maps. In the example above with CCD_ID=4, the extension `AXAF_PCTI_IMAGE4` would be used.

5.2 Required changes

In order to describe the strong changes in temperature, both the format of the CALDB file and the processing in `acis_process_events` have to be changed; however, the changes are relatively minor: The new CTI correction will use the same formulas and equations; it is just that the coefficients are now valid only for a specific temperature range and, when `acis_process_events` selects the row with coefficients, it now needs to select on CCD_ID, CHIP_X, CHIP_Y, **and** temperature.

5.2.1 Changes to the CTI files in the CALDB

The block `AXAF_CTI` will gain three more columns:

1. name: TEMP_LO
   type: Real4
   Range 0:+Inf
   unit: K (degrees Kelvin)
   comment: The lower TEMP boundary where this row is valid

2. name: TEMP_HI
   type: Real4
   Range 0:+Inf
   unit: K (degrees Kelvin)
   comment: The upper TEMP boundary where this row is valid

3. name: TEMP_IND
   type: Int2
   Range -
   comment: Index for third dimension in trap map

The columns in the table used to select the relevant row might look like this (abbreviated example):

```
--------------------------------------------------------------------------------
Data for Table Block AXAF_CTI1
--------------------------------------------------------------------------------

ROW    CCD_ID     CHIPX_LO   CHIPX_HI   CHIPY_LO   CHIPY_HI     TEMP_LO    TEMP_HI   TEMP_IND

     1          0          1       1024          1       1024       148        180           1
     2          1          1       1024          1       1024       151        154           1
     3          1          1       1024          1       1024       154        157           2
     4          1          1       1024          1       1024       157        159.5         3
     5          1          1       1024          1       1024       159.5      165           4
```

The trap maps (fits file extensions AXAF_{S/P}CTI_IMAGE{I}, where S/P identifies serial or parallel CTI, and I is the chip ID) do also depend on temperature. So, their format will be changed to Real4(1024x1024xN) where N can be different for each block. This represents trap maps at different temperatures; the layer is selected by the TEMP_IND column. For a particular CCD, if there is only one trap map for a large range of FP_TEMP available (e.g., the current state of ACIS calibration) then there will only be one TEMP_IND and the value will be equal to 1.

5.2.2 Changes to `acis_process_events`

The equations in `acis_process_events` that use the CTI coefficients or trap maps do not change. However, the appropriate row in the CTI table is now selected on CCD_ID, CHIP_X, and CHIP_Y as before, but also as TEMP_LO <= FP_TEMP < TEMP_HI, where FP_TEMP is the temperature of the focal plane at the time that that particular photon was detected (as recorded in the MTL file). Instead of using the 2D trap map from the appropriate extension, `acis_process_events` selects a 2D slice from the 3-dimensional Real4(1024x1024xN) trap map in that extension. The index for the third dimension is given in TEMP_IND. (Note that we define TEMP_IND with one-based indexing. Depending on the implementation language used in `acis_process_events`, this might have to be translated to zero-based indexing, i.e. the 2D array chosen for a particular photon would be `arr[:, :, TEMP_IND - 1]`.)

In the example above, every photon with CCD_ID=0 will be processed with the coefficients in row 1, but photons on CCD_ID=1 will be processed with coefficient taken from different rows depending on their temperature. A photon with CCD_ID=1 and FP_TEMP=-115.34 C=157.81 K would use the coefficients from row 4. The trap map used will be from block `AXAF_PCTI_IMAGE2`, selecting layer 3 from the array, i.e. `arr[:, :, 3]`.

For backwards compatibility, `acis_process_events` shall make the following assumptions:

- If the new columns are not present, temperature is not used in the column selection.
- In that case, `acis_process_events` shall expect the image extension to have the format Real4(1024x1024) as in CIAO 4.15 and use that trap map as in CIAO 4.15.

5.3 Rationale

This design of the new CTI files does not require the addition of any new files to the CALDB. The temperature range over which a specific set of coefficients is valid can be different by CCD as required by the calibration. In practice, the CCDs used for imaging are likely to be calibrated in smaller temperature bins because the CTI correction is more important for the analysis of imaging observations and more calibration data become available. The changes given here allow for gradual updates of the CALDB as more calibration information is available. Initially, the file can be kept to reproduce the CTI in CIAO 4.15 exactly, simply by having just one row per CCD with settings for TEMP_LO and TEMP_HI that include all temperatures that the ACIS focal plan ever had.

This format is also flexible enough that future changes of the CTI correction can be expressed in this scheme. The CTI correction already implemented in `acis_process_events` (see Ref 3) is a polynomial in temperature. Since any function can be approximated by a polynamial function for small temperature intervals, it is always possible to express any temperature dependence simply by creating many rows in the table and using the already implemented CTI correction as approximation to a more complex function. In that sense, this format is future-proof, even if the needs of the calibration change.

5.4 Backwards and forwards compatibility

The changes are designed to be backwards compatible; a newer version of `acis_process_events` will work with existing CALDB versions, but changes versions of the CALDB would require an updated version of `acis_process_events` in the next DS or CIAO release.