

Sciamachy level 1b patch program

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1 Introduction

This document describes the Sciamachy NRT level 1b pre-processor: *scia_patch_1b*, a software tool that allows you to replace calibration keydata and parameters of a Sciamachy level 1b product (leaving the PDS format intact). *Scia_patch_1b* is written to facilitate further improvement of the calibration of Sciamachy data. This tool is developed for in-house usage and for the Sciamachy validation community to validate the latest developments on the calibration of Scia data. Therefore, this is work in progress, and should be used with care (see section C.1). For advice, please contact the author or the SRON Sciamachy team.

2 SCIA_PATCH_NL1

2.1 Name:

`scia_patch_nl1` – program to patch Sciamachy level 1b products

2.2 Syntax:

`scia_patch_nl1 [OPTIONS] INFILE`

2.3 Description:

`scia_patch_nl1` is a program to test/validate/improve the calibration Sciamachy data by replacing (or patching) several annotation data sets involved in the level 1b to 1c processing. As input it takes a Sciamachy level 1b product (in PDS format) and optionally several auxiliary data sets (described below), the output is a patched Sciamachy level 1b product, also in PDS format.

2.4 Options and Parameters:

- help** print out a message listing of the available options (alternatively: **-h**)
- version** print out version number and copyright information, and exit (alternatively: **-V**)
- silent** do not display any progress messages — info, warning and error messages are always displayed
- o *file_name*** leave the output to file *file_name*, the default is to replace the “Processing stage flag” (= 11th character) by “B”, to indicate that this is a *special* product (alternatively: **-output=*file_name***)
- no_patch** do not apply any patch to the data, only the MPH is modified, see section 2.5.1
- patch[=*0ml,1,3,4,5,6,7,9*]** apply patches to the the data, according to the values entered. For explanation see table 1 [*Default: 0,1,4,5,6,9*].

2.5 Algorithm Description:

2.5.1 Main Product Header (MPH)

Listing of modification are made to the original MPH:

Table 1: Listing of the patch-options, including a brief description.

OPTIONS	SHORT DESCRIPTION
0	same as option 0ml
m	replace memory correction values
l	replace non-linearity correction values
1	replace dark current parameters in CLCP and VLCP GADS (IR channels, only)
2	replace Pixel-to-Pixel Gain in PPG_Etalon GADS
4	replace Straylight correction values of channel 2 in the Science data MDS
5	replace spectral calibration parameters for channel 7/8 in SCP GADS
6	polarization improvements, see appendix A
7	replace Radiance sensitivity values in RSPx GADS
8	replace Solar spectrum values in SRS GADS (<i>not implemented</i>)
9	replace bad pixel mask in PPG_Etalon GADS (IR channels, only)

KEYWORD	MODIFICATION
PRODUCT	replaced by the actual file name
PROC_STAGE	replaced by "B" (= special product)
SOFTWARE_VER	append "pX.XX", where "X.XX" is the patch version

2.5.2 Memory correction [option: 0m]

Description calculate and replace the memory effect correction values. The memory effect only affects detector readouts of the Reticon detectors (channel 1–5), where the signal level of the previous readout has a measurable effect on the current readout (and even on the next readout, but this effect is negligible). The amount of the memory effect has been parametrized for science channels 1–5, based on pre-flight and in-flight measurements and stored in a look-up table.

For non-coadded readouts, the amount of memory effect correction for pixel i in optical channel j is found by using look-up table *MemCorr*:

$$C_{i,j} = MemCorr_j(S_{previous,ij})$$

This value has to be coded as a single signed character on the level 1b product:

$$C_{i,j}(1b) = ROUND(C_{i,j}/2.)$$

In case of coadding, the calculation is slightly more complicated, because only the sum of the signals of all coadded readouts is known, not the individual readouts. As an estimate of the individual readouts, we take the variation of the nearest (in wavelength) PMD signal during the measurement.

For coadded readouts, let $N_{i,j}$ be the number of coaddings per integration time for each detector pixel i in optical channel j . Then we repeat the signal by $N_{i,j}$ (REPLICATE not de-coadd) and calculate the total PMD signals during the detector pixel exposure time ($I_{PMD,PET}$) and during the integration time ($I_{PMD,Intg}$). The variation of the PMD signal during the measurement $m \in [0, N_{i,j}]$ is then obtained as follows:

$$W_{PMD,PET}(m) = \frac{I_{PMD,PET}(m)}{I_{PMD,Intg}}$$

Then the (repeated) individual signals are multiplied by $W_{PMD,PET}$, and the memory effect correction of individual measurement m is:

$$C_{i,j}(m) = MemCorr_j(W_{PMD,PET}(m) * S_{previous,ij}(m))$$

The total memory effect correction for the coadded signal is given by:

$$C_{i,j} = C_{previous,i,j}(N_{i,j} - 1) + \sum_{n=1}^{N_{i,j}-1} C_{i,j}(n - 1)$$

Remark 1: negative PMD values are replaced by zero

Remark 2: the SciaLIC applicator (version $i = 2.3.x$) should apply the memory correction correctly. However, the scale factor and offset are likely to be replaced in the near future by 1.25 and -37 respectively.

Auxiliary data HDF5 file with a look-up table containing the memory correction value as function of measured signal. File: DATA_DIR/MEMCORR.h5

Reference SRON-SCIA-PhE-RP-11

Status implemented

2.5.3 Non-linearity correction [option: 0]

Description calculate and insert correction values for non-linear behavior of the Sciamachy infra-red science detectors, based on measurements made during OPTEC5. The Sciamachy Epitax science detectors show non-linear behavior, in contrast to the Reticon detectors. This effect can introduce errors on the science measurements of up to 200 BU. The non-linearity correction is based on average correction curves for specific sub-divisions of pixels within a physical channel. The sub-divisions consists of four channels (6, 6⁺, 7 and 8), two multiplexers (odd and even) and two sub-channels (lower and higher than pixel 511). The accuracy of the curves seems to be adequate, a maximum systematic error is expected of 5% at 25 kBU, and this only for channel 8.

For non-coadded readouts, the non-linearity effect correction for pixel i in channel j ($j \in [6, 8]$) is found by using two look-up tables. One to find the right curve: *Curve* and a second with the correction values: *nLinCorr*:

$$C_{i,j} = nLinCorr[S_{i,j}, Curve_{i,j}]$$

This value has to be coded as a single signed character on the level 1b product:

$$C_{i,6}(1b) = -102 + ROUND(C_{i,6}/1.25)$$

$$C_{i,7}(1b) = -126 + ROUND(C_{i,7}/1.5)$$

$$C_{i,8}(1b) = -126 + ROUND(C_{i,8}/1.25)$$

In case of coadding, the calculation is slightly more complicated, because only the sum of the signals of all coadded readouts is known, not the individual readouts. As an estimate of the individual readouts, we take the variation of the nearest (in wavelength) PMD signal during the measurement.

For coadded readouts, let $N_{i,j}$ be the number of coaddings per integration time for each detector pixel i in optical channel j . Then we repeat the signal by $N_{i,j}$ (REPLICATE not de-coadd) and calculate the total PMD signals during the detector pixel exposure time ($I_{PMD,PET}$) and during the integration time ($I_{PMD,Intg}$). The variation of the PMD signal during the measurement $m \in [0, N_{i,j}]$ is then obtained as follows:

$$W_{PMD,PET}(m) = \frac{I_{PMD,PET}(m)}{I_{PMD,Intg}}$$

Then the (repeated) individual signals are multiplied by $W_{PMD,PET}$, and the non-linearity effect correction of individual measurement m is:

$$C_{i,j}(m) = nLinCorr[W_{PMD,PET}(m) * S_{i,j}(m), Curve_{i,j}]$$

The total non-linearity effect correction for the coadded signal is given by:

$$C_{i,j} = \sum_{n=0}^{N_{i,j}-1} C_{i,j}(n)$$

Remark 1: the non-linearity correction values are only valid for readouts in the range between 0 BU and 60,000 BU.

Remark 2: negative PMD values are replaced by zero in the calculation of the non-linearity correction.

Remark 3: the SciaL1C applicator (version $\leq 2.3.x$) ignores the non-linearity values in the patched level 1b products

Auxiliary data HDF5 file with a look-up table containing non-linearity correction as function of measured signal. File: DATA_DIR/NLcorr.h5

Reference SRON-SCIA-PhE-RP-013

Status implemented

2.5.4 Darkcurrent correction [option: 1]

Description replace the variables FPN and LC (channel 6–8) in the GADS “LEAKAGE_CONSTANT” by values derived from the daily measured darks. The analog offset and dark current values are derived from dark measurements (StateId’s 8, 26, 46, 63, and 67) by default. When these states are not available, Nadir eclipse measurements (StateId 1) or ADC (StateID 65) measurements are used as an alternative. All data is corrected for memory effect (channel 1–5) and non-linearity (channel 6–8) prior to further processing.

The darksignal of channel 7 and 8 show some orbital variation due to small temperature variation of Sciamachy optical bench module. This variation is mainly noticed in channel 8, and obscured in channel 7 by a light leak. The orbital variation of channel 8 is derived from monthly dedicated calibration orbits in which only dark measurements are performed. The orbital variation is corrected for transmission loss due to the ice layer. The orbital variation values are written to the GADS “LEAKAGE_VARIABLE”.

Remark 1: the dark correction values are read from the Monitoring database. The algorithm to select dark signal parameters from the database searches for the first entry (i.e. with a minimal difference in orbit number), where the *quality* ≥ 70 . The maximum allowed difference in orbit number, for a solution, is 21. When within this range no entry is found with the required *quality* then the entry with the highest *quality* (> 40) is used. Note that, due to this restriction, the dark current values are not always replaced.

The *quality* of the derived dark signal parameters is based on the number of unique dark state-id’s found in a Level 0 product:

Quality	Number of unique dark State-id’s
-1	none
40	ADC
50	South Pole dark
70	2
80	3
90	4
100	5

Remark 2: Before orbit 3066 (2002/10/01): only sparse execution of 2 or 3 darks states in some time lines. Between orbits 3066 and 4152 (2002/12/16): each orbit contains 3 blocks of 3 darks from which accurate dark signal parameters can be derived. Between orbits 4153 and 5713 (2003/12/16): each orbit contains 2 blocks of 5 darks. Orbit 5714 and later: each orbit contains 3 blocks of 5 dark states to enable a more accurate modeling of the orbital variation of the dark signal within a single orbit.

Remark 3: the orbital variation correction values are read from the Monitoring database. The algorithm to select orbital variation correction values uses a search radius of 42 orbits. Note that, due to this restriction, the orbital variation correction values are not always replaced.

Auxiliary data the analog offset and dark current are read from a binary file (Little-endian, one file per orbit) in the directory: `DATA_DIR/DarkCurrent`.

The orbital variation function for the ice-free detector is derived from a fit to a data set of monthly dark calibration orbit covering a large orbit range. This orbital variation function is rather constant in time, and updated only occasionally. The orbital variation function is regularly (daily) corrected with the transmission of the ice-layer obtained from the Sun over ESM diffuser measurements. The orbit phases are given per $1/72$ of an orbit. The orbital dark signal is read from a binary file (Little-endian) in the directory: `DATA_DIR/OrbitalVariation/Transmission` containing one float array(1024,72) with the correction (only for channel 8).

Reference SRON-SCIA-PhE-RP-012 and SRON-SCIA-PhE-RP-018

Status implemented

2.5.5 Pixel-to-Pixel gain correction [option: 3]

Description replace Pixel-to-Pixel Gain in PPG.Etalon GADS

Auxiliary data

Reference None

Status implemented/experimental

2.5.6 Straylight correction [option: 4]

Description replace Straylight correction values of channel 2 in the science data MDS

Auxiliary data HDF5 file with a look-up table containing the Straylight correction matrix.
File: `DATA_DIR/Straylight.h5`

Reference RESULTS OF A NEW STRAYLIGHT CORRECTION FOR SCIAMACHY *Sander Slijkhuis(1), Ralph Snel(2), Bernd Aberle(1), Günter Lichtenberg(1), Markus Meringer(1), Albrecht von Bargaen(1)*

Status implemented

2.5.7 Spectral Calibration Parameters (chan 7/8) [option: 5]

Description replace wavelength of detector pixels in GADS "SPECTRAL_BASE". *Outdated, already implemented in the Operational processor since version 4.x (TBC)*

Auxiliary data the precise basis array of wavelength values for channels 7 and 8 is calculated using 2 polynomials for channel 7 and 8, resp.:

$$1934.376 + 0.117475 * px - 1.04148e - 5 * px^2$$
$$2259.237 + 0.135254 * px - 1.19719e - 5 * px^2$$

Reference SRON-EOS-HS-00001

Status implemented

2.5.8 Polarization improvements [option: 6]

Description A detailed description of the problem is described in Appendix A. The patch software applies the three suggested and approved corrections for the Stokes parameters Q and U. *Outdated, already implemented in the Operational processor since version 5.04 (TBC)*

Auxiliary data none

Reference see Appendix A

Status implemented

2.5.9 Absolute Radiance [option: 7]

Description replace the radiance sensitivity parameters in the GADS “RAD_SENS_NADIR”, “RAD_SENS_LIMB” and “RAD_SENS_OCC”

Auxiliary data HDF5 file with the radiance sensitivity parameters as derived from the “operation keydata”, used for the Verification data sets Feb. 2005. File: DATA_DIR/rsp_patch.h5

Reference IFE-SCIA-SN-20050203_IrrRadCorrection

Status implemented

2.5.10 Solar spectrum [option: 8]

Description replace the Solar spectrum in the GADS “SUN_REFERENCE”.

Auxiliary data database with Solar measurements, corrected for memory effect and non-linearity, stored as binary file (Little-endian) in the directory: DATA_DIR/SunStates. The format of the file: ...

Reference TBS

Status under development

2.5.11 Bad pixel mask [option: 9]

Description replace bad pixel mask in the GADS “PPG_Etalon” with a smoothed bad pixel mask. First, for each Level 0 file an orbital bad pixel mask is determined. Several diagnostics are available to detect bad pixels: noise, analog offset (error), dark current (error), chi-square of the dark current fit, residual of the dark measurements after dark correction, WLS- and Sun-response, and pixel-to-pixel gain. The thresholds on these parameters are specified independently for each channel, treating channel 6 and channel 6+ separately. The bad pixel mask that is patched into the Level 1b product is smoothed using the orbital bad pixel masks from the 50 previous orbits, after filtering on dark-quality and SAA flag. In case WLS- and Sun-response masks are not included in the averaging window, the most recent valid WLS- or Sun-response mask is added. The Pixel-Gain mask is averaged over the last 15 available valid Pixel-Gain masks.

Auxiliary data the smoothed bad pixel mask is read from an ASCII file (one file per orbit) in the directory: DATA_DIR/SmoothMask/ASCII. Each file contains a table with one column and 8196 rows holding an integer flag: 0 = ok, 1 = Bad.

Reference SRON-SCIA-PhE-RP-21

Status implemented

A Polarisation Improvements (J.M. Krijger, SRON)

A.1 Introduction

SCIAMACHY measures the polarisation Stokes parameters Q and U at several wavelengths with PMDs. Stokes parameters Q and U are needed for radiometric calibration of SCIAMACHY, because the instrument is sensitive to polarised light. Good polarisation correction is essential for many SCIAMACHY level 1 and level 2 products. Verification of Q and U is done by comparison with polarised radiative transfer model calculations and analytical expressions for single Rayleigh scattering (Tilstra et al., 2002). The main focus is on nadir polarisation validation.

A.2 Changes

At this moment (Feb 2004) several (three) suggested and approved corrections have not yet been implemented in the operational Level-0-to-1 dataprocessor. These three corrections concern:

A.2.1 PMD 4 & 7 Unphysical

PMD 7, also known as PMD₄₅, is the only PMD measuring U-polarisation and covers approximately the same wavelength range as PMD 4, which measures Q-polarisation. For unknown reason (though wrong calibration is suspected and under investigation) the combination of these PMDs produces unphysical results. In order to avoid clearly wrong polarisation correction this PMD combination should not be taken into account for the polarisation interpolation and/or correction.

A.2.2 Incorrect U/Q ratio

The measured U/Q ratio derived from the combination of PMD 4 & 7 is used to derive the U-values for PMD 3,5 & 6. As the PMD 4 & 7 combination does not produce physical polarisation values, their ratio is also unphysical. This leaves the U-values from PMD 3,5 & 6 clearly wrong. The best method (which will be used in the future) is to derive Q and U by using the (by viewing geometry dictated) U/Q ratio derived from theoretical Rayleigh single scattering. We have only corrected U here, as the correction on Q is only possible in a complete recalculation of level-0-to-1b. The U-values of PMD 3,5 have been replaced by:

$$u_i = \text{sign}(u_0) \cdot \left(|q_i \cdot u_0 / q_0| \leq \sqrt{(u_0^2 + q_0^2 - q_i^2)} \geq 0 \right) \quad (1)$$

with u_0 and q_0 being the respective u and q value derived from single scattering and u_i and q_i the respective u and q value we are interested in. The latter part of the equation is to keep U within physical boundaries ($U \leq U_0$ and $\sqrt{u^2 + q^2} \leq \sqrt{u_0^2 + q_0^2}$).

A.2.3 Infrared (PMD 6) Unphysical

At this moment PMD 6 produces unphysical results due to the ice problem, the noise on the measurements and the unknown correction needed for the non-overlap with the main channels. This problem is not expected to be solved within the near future and thus, in order to avoid incorrect polarisation corrections, all U and Q values from this PMD are put to zero, as little polarisation is expected at infrared wavelengths.

A.3 Discussion

To summarise:

- PMD 4&7 combination is not used for polarisation correction purposes.
- The U-values for PMD 3&5 are replaced with their Q-values multiplied with their theoretical Rayleigh single scattering U/Q ratio.
- PMD 6 U and Q-values are put to zero.

While these corrections are not perfect and still leave (small) errors, they strongly improve the quality of the polarisation correction.

B Auxiliary calibration data sets

All auxiliary calibration datasets are search (first) in the current directory and (secondly) in the directory `DATA_DIR`. The value for `DATA_DIR` is set in the configuration file `config/Rules_NADC.mk`, and thus fixed during the compilation of `nadc_tools`.

B.1 Memory correction dataset

The memory correction values are written from a HDF5 file with a lookup table containing the correction value as function of measured signal. The name of the file: “MEMcorr.h5”, its content is described in the table below:

Dataset	Type	dimensions
MemTable	float	5, 65536

B.2 Non Linearity correction dataset

The non-linearity correction values are written from a HDF5 file with a lookup table containing the correction value as function of measured signal. The name of the file: “NLcorr.h5”, its content is described in the table below:

Dataset	Type	dimensions
CurveIndex	signed char	8, 1024
nLinTable	float	15, 65536

B.3 Dark current correction datasets

The analog offset and dark current values are read from a binary file: Little-endian, one file per orbit. Given are several parameters in the DarkCurrent records, see table below: Applicable files are searched in the directory: `DATA_DIR/DarkCurrent`.

Dataset	Type	dimensions
Orbit	long	1
MagicNumber	long	1
Saa	long	1
Time	double	1
Tobm	float	1
Tdet	float	8
QualityNumber	long	1
AnalogOffset	float	8192
DarkCurrent	float	8192
AnalogOffsetError	float	8192
DarkCurrentError	float	8192
ChiSquare	float	8192

The orbital variation of the darksignal is read from a binary file: Little-endian, one file per orbit. Given are the correction, only for channel 8 for 72 orbit phases, starting at orbit phase 0. The format of the file binary, containing one float array of dimension: 1024, 72 Applicable files are searched in the directory: `DATA_DIR/OrbitalVariation/Transmission`.

B.4 Radiance sensitivity correction dataset

The Radiance sensitivity values are written from a HDF5 file. The name of the file: “rsp_patch.h5”, its content is described in the table below:

Dataset	Type	dimensions
KEY_DATA_FILE	string	62
/RSPL/azimuth	float	115
/RSPL/elevation	float	115
/RSPL/sensitivity	float	115, 8192
/RSPN/azimuth	float	17
/RSPN/elevation	float	17
/RSPN/sensitivity	float	17, 8192
/RSPO/azimuth	float	45
/RSPO/elevation	float	45
/RSPO/sensitivity	float	45, 8192

B.5 Dead and Bad pixel mask datasets

The bad pixel mask is read from an ASCII file: one file per orbit. Each file contains a table with one column and 8192 rows holding an integer flag: 0 = ok, 1 = Bad. Comment-lines are indicated with an #, as first character. Applicable files are searched in the directory: DATA_DIR/SmoothMask/ASCII.

C About NADC tools

C.1 Purpose and Limitations

The probably most important part of the NL-SCIA-DC software (`nadc_tools`) are the C-libraries, which contain functions to read Sciamachy data products into memory, dump the data as ASCII output or write the data in PDS or HDF5 format. The software is written in ANSI-C (and even assembler), and coded in such a way that you (an experienced (C-) programmer) can easily understand the code. The data extractors, included in this software package, are developed for the NL-SCIA-DC and give a good example of how to use the libraries.

The software distributed in this package contains libraries, written in ANSI-C (mostly POSIX compliant except for some ISO C99 extensions) and an IDL wrapper library (using `CALL_EXTERNAL`) with IDL functions to read GOME and Sciamachy data. The IDL interface requires sharable object libraries. Building shared libraries is easy on the supported platforms, however, do not forget to set the environment variable `LD_LIBRARY_PATH`.

This software package is written and maintained by Richard van Hees (SRON), and distributed under the GNU General Public License.

C.2 Acknowledgement

In case (part of) this dataset is used for a publication and essential to the work and the results, an offer of co-authorship to Richard van Hees (SRON) and /or Ralph Snel (SRON) is highly appreciated. Please do not hesitate to contact us in an early stage for necessary support.

In all other cases SRON should be properly acknowledged. Such an acknowledgement could state: “We acknowledge SRON for providing the `nadc_tools` and/or patched Sciamachy level 1b data products”.

C.3 DISCLAIMER

We at SRON have developed `nadc_tools` as part of our commitment towards the verification and further improvement of the calibration of Sciamachy data. This software is developed for in-house usage, and generously shared with you **WITHOUT ANY WARRANTY**. We will try to help you with any problems, but only on a “best effort” basis. In order to continuously improve this facility, feedback from users is highly appreciated.

Note that this software package is also not supported in any way by ESA or DLR, although the `nadc_tools` extractors and libraries mimic some of the functionality of the `gdp` and `Enviview` toolbox.

The software package is in no way intended to replace the official data processor and should not be treated as such. Especially it is not meant to (and cannot) produce official data products. These have to be derived with ESA approved tools such as `Enviview` that can be downloaded for free from ESA.

It is your own responsibility to verify the results you produce with this package against official data products. If you find discrepancies, please inform SRON (not ESA or DLR) at once. Any information you give will help us to improve our software. We will relay to ESA all information to improve the official data processor.

C.4 COPYRIGHT

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