Sentinel-3 SLSTR Uncertainties in Level-1 Products Algorithm and Theoretical Basis Document

	Name	Signature / Date
Prepared By	**Mireya Etxaluze**	Mireya Etxaluze 2019.10.28 09:35:44 Z
Checked By	**Dave Smith**	Dave Smith 2019.10.25 13:24:21 +01'00'

Science and Technology Facilities Council
Rutherford Appleton Laboratory
Harwell Science and Innovation Campus
Didcot
Oxfordshire OX11 0QX
United Kingdom

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CHANGE LOG

Date	Issue	Revision	Pages	Reason for change
11-Apr-2019	1	0		Creation
04-Sep-2019	2	0		RIDs from EUMETSAT included
25-Oct-2019	3	0		- Potential Evolutions included - Output file name changed to <b>_ uncertainties _<g><v>.nc as requested in RIDs Typographical corrections

CONTENTS

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1 Scope of Document / Introduction

This document describes the theoretical justification for the algorithm developed to allow the estimates of the SLSTR Level-1 random noise (NEΔT and NEΔL) and correlated uncertainties (uBT, uL) in the radiometric calibration to be mapped for each L1 image pixel. This work has been performed under the European Union's Copernicus Programme, and managed by EUMETSAT through the contract EUM/CO/18/4600002122/AOC.

2 Terms, Definitions and Abbreviations

2.1 Terms and Definitions

Channel- Spectral channel (S1-S9 + F1-F2)

Calibration is the process of quantitatively defining the system response to known, controlled system inputs.

Error is defined as the difference between a result obtained and the 'true' value.

Field-Of-View - is the angular extent of a given scene that is viewed by the instrument.

Infrared (IR) radiation is electromagnetic radiation of wavelengths between about 750nm and 1mm. This is broken down into 5 wavelength regions

Near-IR - 0.75-1.4 µm

Short-Wave IR - 1.4-3 µm

Medium-Wave IR - 3-8 µm

Long-Wave IR - 8–15 µm

Image swath - Maximum distance on ground between the positions of two spatial samples belonging to the same row.

Image sample - image element containing radiance measurements of co-registered pixels for all bands.

Precision is defined as the difference between one result and the mean of several results obtained by the same method.

Traceability is the property of the result of a measurement or the value of a standard whereby it can be related to stated references, usually national or international standards, through an unbroken chain of comparisons all having stated uncertainties.

Uncertainty parameter associated with the result of a measurement, that characterises the dispersion of the value that could reasonably be attributed to the measurand.

Type A evaluation (of uncertainty) method of evaluation of uncertainty by the statistical analysis of series of observations. This is usually given by the standard deviation of a number of measurements of a variable.

Type B evaluation (of uncertainty) method of evaluation of uncertainty by means other than the statistical analysis of series of observations. This is usually based on existing knowledge, for example

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data provided in calibration and other certificates or an estimation of the uncertainty based on previous experience.

Visible light is electromagnetic radiation detectable by the human eye with a wavelength between approximately 400nm and 700nm.

Validation is the process of assessing by independent means the quality of the data products derived from the system outputs.

2.2 Acronyms

AATSR	Advance Along-Track Scanning Radiometer
ADC	Analog-to-Digital Converter
ADF	Auxiliary Data File
ATBD	Algorithm Theoretical Basis Document
BB	Blackbody
BT	Brightness Temperature
CPU	Central Processing Unit
GPP	Ground Prototype Processor
IODD	Input Output Data Definition
IPF	Instrument Processing Facility
IR	Infrared
LUT	Lookup Table
NetCDF	Network Common Data Format
NEΔL	Noise Equivalent Differential Radiance
NEΔT	Noise Equivalent Differential Temperature
RAL	STFC Rutherford Appleton Laboratory, UK
SLSTR	Sea and Land Surface Temperature Radiometer
STFC	Science and Technology Facilities Council
SRD	System Requirements Documents
SWIR	Short-Wave Infrared
TIR	Thermal Infrared
VIS	Visible
VISCAL	Visible Calibration Unit

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3 Documents

3.1 Applicable Documents

The applicable documents are:

	Document title	Document reference
AD1	SLSTR PFMr TIR Channel Calibration Report	S3-RP-RAL-SL-122
AD2	SLSTR Level-1 ATBD	S3-TN-RAL-SL-032
AD3	Sentinel-3 Product Data Format Specification SLSTR Level 1 & Level 2 Products	S3IPF.PDS.005
AD4	Sentinel-3 Core PDGS Instrument Processing Facility (IPF) Implementation. Auxiliary Data Format Specification	S3IPF.PDS.007
AD5	PFMr VIS and SWIR Calibration Report	S3-PR-RAL-SL-121
AD6	ESA GMES Sentinel-3 System Requirements Document, Issue 4	S3-RS-ESA-SY-0010
AD7	SLSTR B FPA Spectral Calibration Report	S3-PR-RAL-SL-102

3.2 Reference Publications

RP1	**Book**	**Editor**	**Publisher**
	Intelligent Production Machines and Systems	John T. Sample & Elias Ioup	Elsevier
	Title	**Author**	**Year**
	Spectral Characterization of digital Cameras using Genetic algorithms	Ioannis Chatzis, Dimitris Gavrilis, Evangelos Dermatas	2006

RP2	**Title**	**Author**	**Reference**
	The Sea and Land Surface Temperature Radiometer (SLSTR) Detection Assembly design and performance	P. Coppo, C. Mastrandrea, M. Stagi, et al.	SPIE, Remote Sensing, 2013

RP3	**Title**	**Author**	**Reference**
	Traceability of the Sentinel-3 SLSTR Level-1 Infrared Radiometric Processing	D. Smith, S. Hunt, E. Wooliams et al.	In preparation

RP4	**Title**	**Author**	**Reference**
	Applying principles of metrology to historical Earth observations from satellites	J. Mittaz, C.J. Merchant, E.R. Woolliams	Metrologia 56, 2009

RP5	**Title**	**Author**	**Reference**
	D2-2a: Principles behind the FCDR effects table	E. Woolliams, et al.	Technical report. National Physical Laboratory and University of Reading. 2017

3.3 Objectives

This document presents the algorithms to allow users of SLSTR Level-1 data to derive per pixel uncertainty estimates using the information contained in the Level-1 products, and additional auxiliary data files (ADF). The per-pixel uncertainty information is provided in complementary datasets that are generated. The algorithm can either be applied directly by users (by provision of a user tool) or implemented as an upgrade to the IPF processor.

4 Algorithm Definition

The Level-1 quality data sets contain estimates of the random signal noise (NEΔT and NEΔL) per scan line derived from the on-board calibration sources, and correlated radiometric uncertainties as a function of scene brightness temperature/radiance derived from the pre-launch calibration.

The algorithm requires a combination of uncertainty estimates data provided in the Level-1 products and some additional parameters derived from the pre-launch calibration contained in Level-1 and Level-2 ADFs.

As part of this work, an article for publication is being written, where the calibration model and the uncertainty contributions are presented in detail [RP3].

The noise derived from the on-board calibration sources is an uncertainty associated with fully random errors. Fully random errors vary unpredictably from measurement to measurement. These errors are entirely uncorrelated between measurements and can be reduced by averaging [RP4, RP5].

The radiometric uncertainty is associated with correlated errors arising from the pre-launch calibration [RP4, RP5].

Figure 1 shows graphically a description of the algorithm. The noise is estimated for both, for the TIR channels and for the solar channels. The script provides NEΔL for the solar channels and NEΔT for the TIR channels. In addition, the output NetCDF file for TIR channels contain the dL/dT values, which can be used by the user to transform NEΔT into NEΔL.

The naming convention of the input data is described in Table 1 using the place holders for the satellite, band, view and grid names, which are to be substituted for each valid combination.

A limitation of the current Level-1 data quality information is that noise estimates are only provided from the two on-board blackbodies. For the TIR channels (S7-S9, F1-F2) NEΔT values are provided for two scene temperatures. For the VIS/SWIR channels (S1-S6) only dark noise estimates are provided. A radiometric noise model is applied to these data to provide noise estimates for the full range of scene BT/radiances.

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Table 1 Abbreviation meaning of the place holders for the satellite, band, view, and grid names for SLSTR channels

Variable	Place holder	Possible Values
Mission ID	<MMM>	– S3A or S3B
band	<b>	– S1 to S6 for VIS/SWIR – S7 to S9 for TIR – F1, F2 for Fire channels
view	<v>	– ‘n’ for nadir view – ‘o’ for oblique view
grid	<g>	– ‘a’ for 0.5km visible and SWIR “A stripe” grid – ‘b’ for 0.5km SWIR “B stripe” grid – ‘i’ for 1km TIR or Fire channels grid

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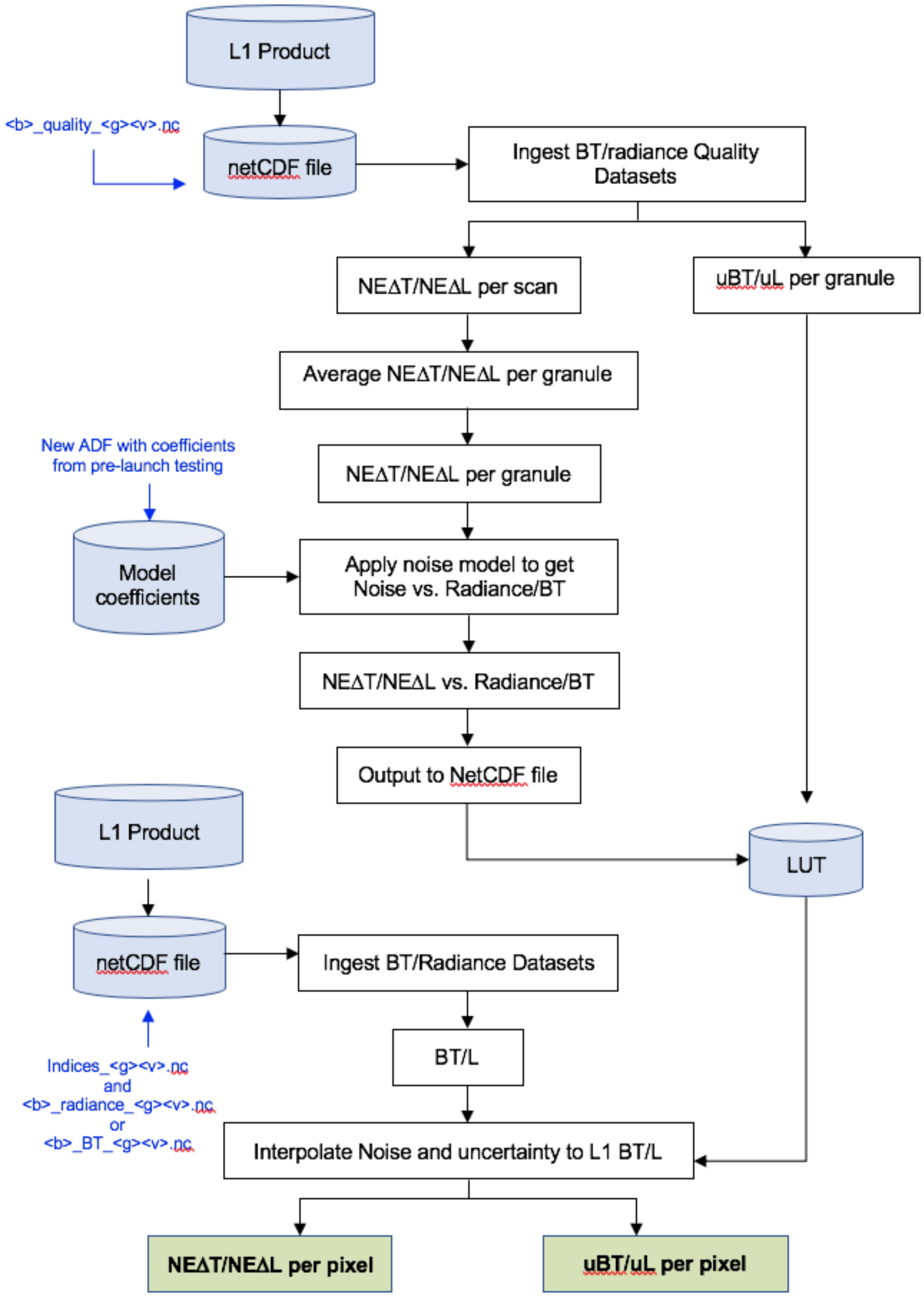

Figure 1 Diagram of the proposed algorithm to map L1 uncertainties for each pixel. The script provides NEDL, uL for the solar channels and NEDT, uBT for the TIR channels. In addition, the output NetCDF file for TIR channels contain the dL/dT values, which can be used by the user to transform the uncertainties from temperature to radiance units if needed .

5 Algorithm Description for TIR/Fire Channels

The algorithm requires SLSTR Level-1 product package and auxiliary data files (ADF). Only the data files required for the algorithm performance are described here.

5.1 Input Files for TIR channels

Figure 2 shows a diagram of the input files necessary for the estimate of the Level-1 uncertainties at the pixel level.

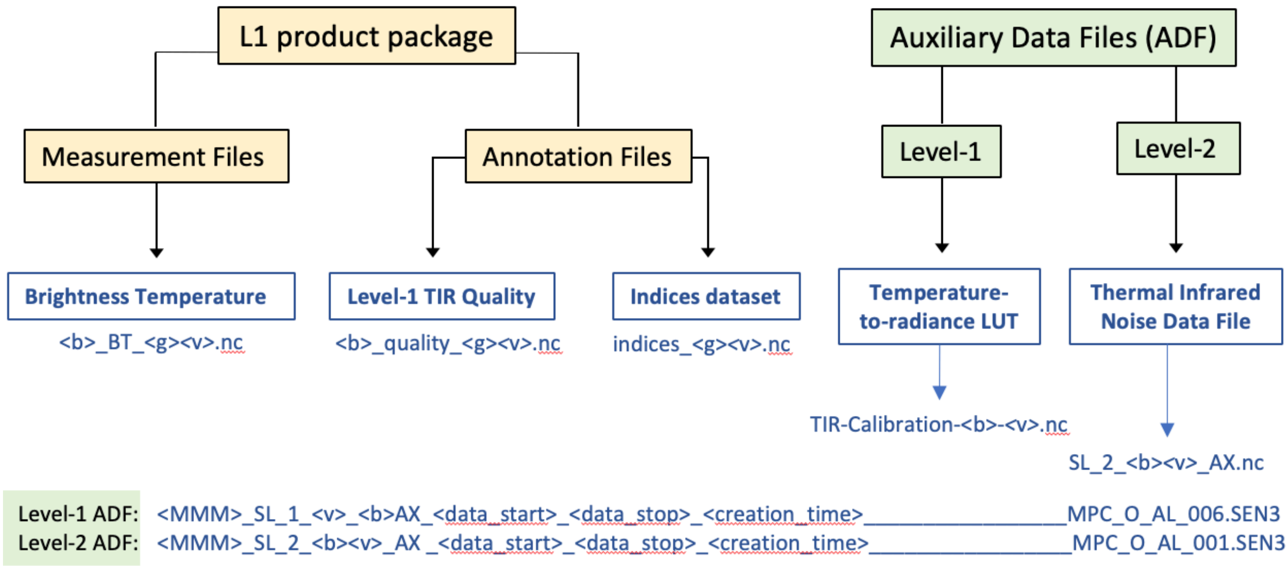

Figure 2 Algorithm input files for TIR Channels

The sources of information needed to perform the mapping of uncertainty estimates are described below

1) The SLSTR Level-1 product which is composed of several NetCDF files containing the different measurement and annotation data sets, including:

   a) The measurement datasets comprising the brightness temperature for each thermal infrared channel S7 to S9 and each fire channel F1 and F2, sampled at 1 km resolution on a quasi-cartesian image grid. These files are:

      <b>_BT_ <g><v>.nc

   b) The annotation files contain Level-1 Thermal Infrared Quality data files:

      <b>_quality_<g><v>.nc

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These files contain estimates of detector noise measured from the blackbody signals, and the LUT of radiometric calibration uncertainty estimates.

An indices dataset containing the scan, pixel and detector number of the image pixel in the original instrument coordinates.

indices_<g><v>.nc

2) The SLSTR Level-1 TIR ADF used in the Level-1 processing. The file identification is:

<MMM>_SL_1_<v>_<b>AX_<data_start>_<data_stop>_<creation_time>_MPC_0_AL_001.SEN3

The file contains NetCDF files with the name

updated_v3_<MMM>_SL_CCDB_CHAR_TIR-Calibration-<b>-<v>.nc

that contains temperature-to-radiance lookup tables (blackbody emissivity and non-linearity LUT).

Note: These files are not provided with the Level-1 product.

3) SLSTR Level-2 ADF

<MMM>_SL_2_<b><v>_AX__<data_start>_<data_stop>_<creation_time>_MPC_0_AL_001.SEN3

This file contains a NetCDF file with the name

SL_2_<b><v>_AX.nc

which contains a LUT of detector noise as a function of scene temperature and detector temperature. The purpose of this file is to provide a reference curve that allows the NEΔT values at the two on-board bb temperatures provided in the quality datasets to be scaled as a function of scene temperature. The current version of the Level-2 auxiliary files were defined during the original GPP (Ground Prototype Processor) development from AATSR measurements and do not represent the actual behavior of SLSTR. For this tool we propose a new, simpler auxiliary file with the noise values vs. temperature.

5.1.1 Level-1 Brightness Temperature Data

The calibrated brightness temperatures from each instrument pixel are mapped onto a regular quasi-cartesian grid with a resolution ~1km for the thermal IR and fire channels. The measurement datasets are contained in the files:

<b>_BT_<g><v>.nc

Figure 3 shows a typical S3A SLSTR Level-1 Brightness Temperature product observed on the 31st May 2018 (orbit 377). The size of the image is 1441x1200 pixel^2 and 810x1200 pixel^2 for nadir and oblique view, respectively.

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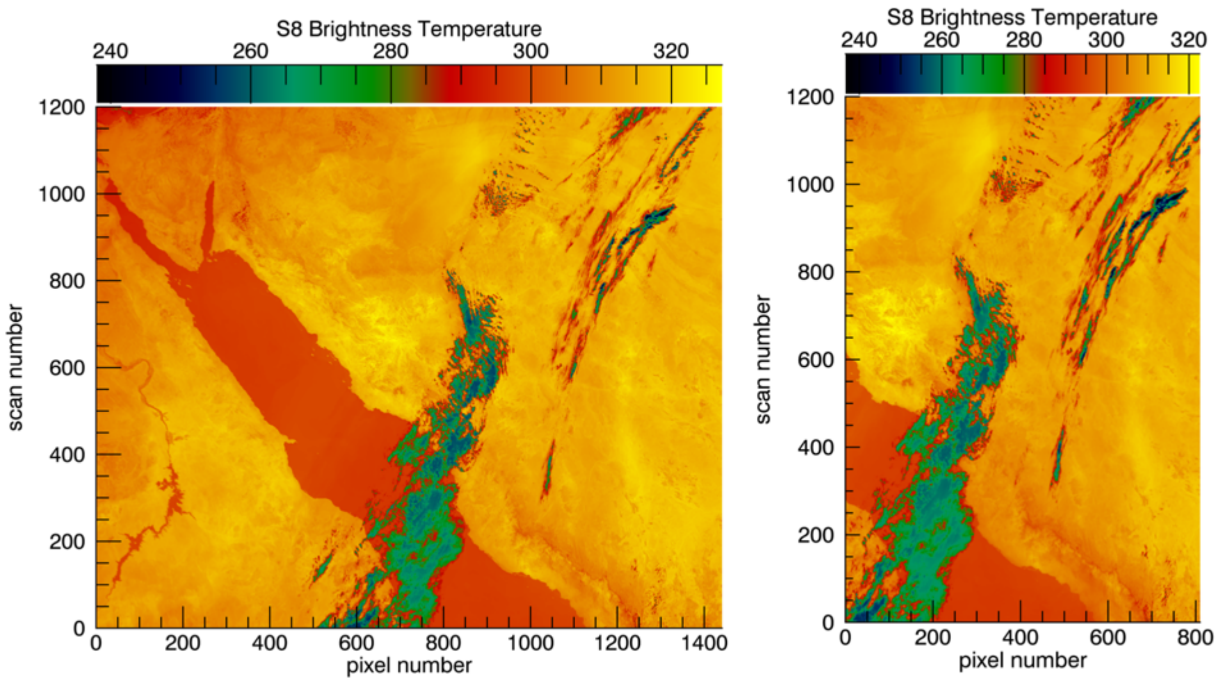

Figure 3: Brightness Temperature map over Red Sea as observed by channel S8 in nadir (left) and oblique (right) views

5.1.2 Radiometric Uncertainty

The Level-1 quality products contain a LUT with correlated uncertainty estimates in the radiometric calibration as a function of scene temperature. The key parameters in the LUT are:

<b>_scene_temperature_<g><v> = LUT Abscissa values
<b>_radiometric_uncertainty_<g><v> = LUT Ordinate values

The calibration uncertainties were derived during the pre-launch calibration using the calibration budget described in the pre-launch calibration report [AD1]. Note that the uncertainty is not a single value (as in the uncertainty is 0.1K) but it is dependent on the scene temperature.

Figure 4 shows the IR channel radiometric calibration uncertainty estimates provided in the current Level-1 product as a function of the scene brightness temperature.

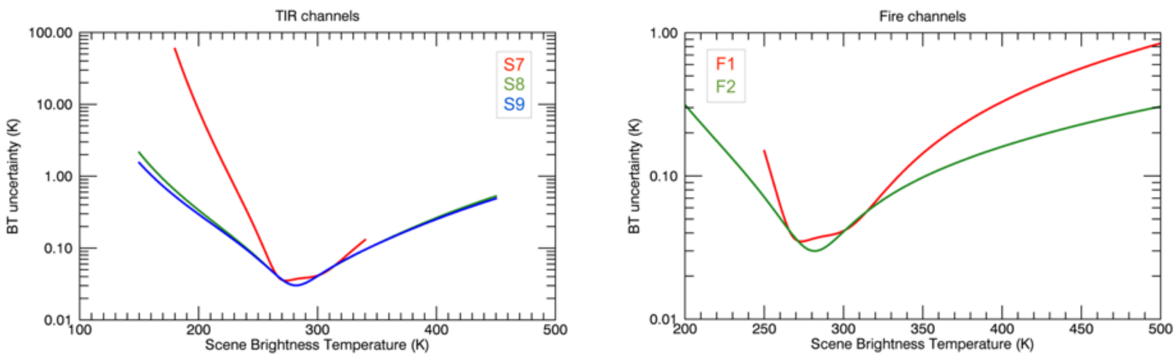

Figure 4: Radiometric uncertainty as a function of scene temperature for the TIR channels (left) and Fire channels (right)

5.1.3 NE∆Ts at BB Temperatures

The radiometric quality datasets contain the noise equivalent temperature differences (NE∆T) in K for each scan line of the image. The noise is a fully random uncertainty provided for each scan line, integrator and detector. The derivation of the radiometric noise is provided in the Level-1 ATBD [AD2].

Figure 5 and Figure 6 show the Hot and the Cold blackbody temperature measure per scan, and the measured NE∆T per scan by each detector, respectively. The variation of the Hot and the Cold blackbody temperature measured per scan along the granule is less than 1 mK.

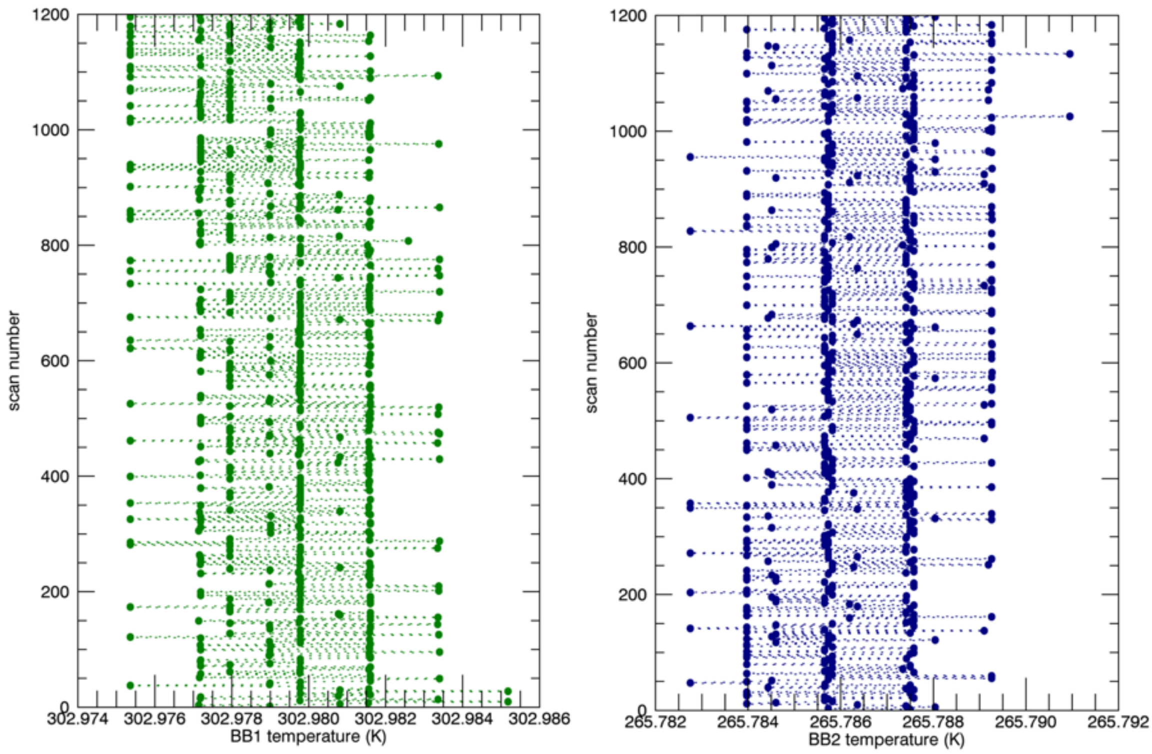

Figure 5: Temperature measured by the Hot (Left) and the Cold (right) blackbodies over each scan.

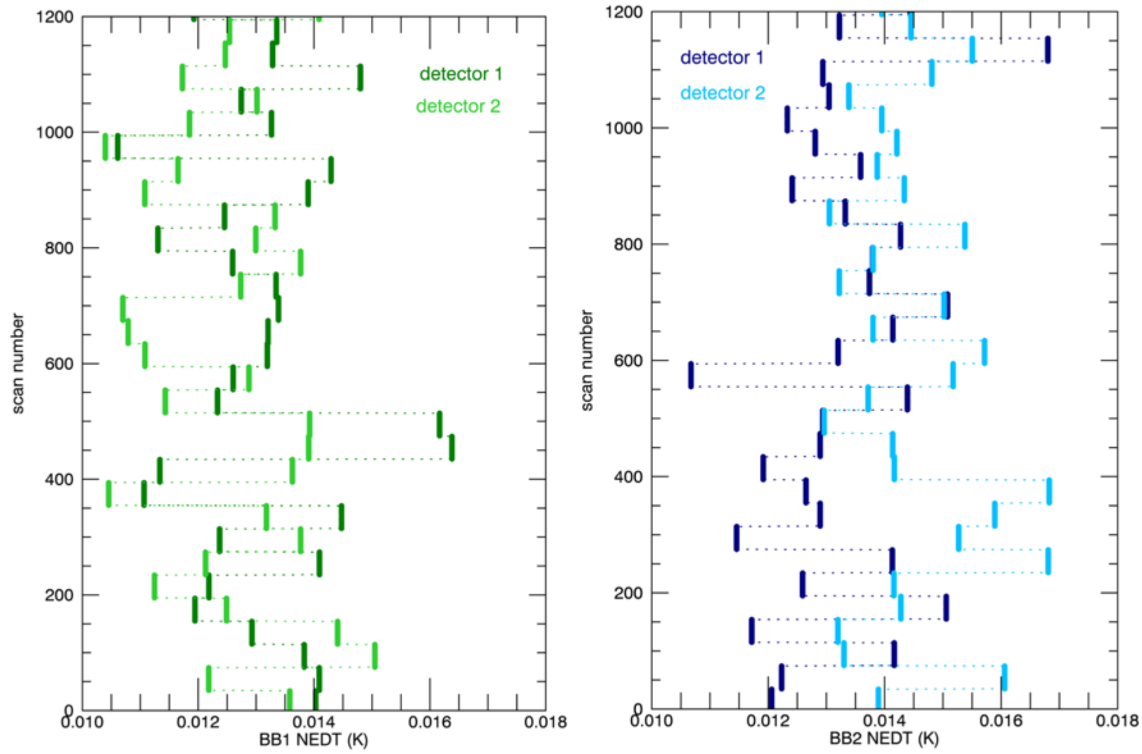

Figure 6 NEΔT per scan determined over the Hot (Left) and the Cold (right) blackbodies.

5.1.4 Temperature-to-Radiance LUT

The temperature-to-radiance LUT in the Level-1 calibration ADFs provides the in band spectral radiance as a function of temperature from 77K to 330K for S7-S9, and from 200K to 500K for F1 and F2. Figure 7 shows the temperature to radiance LUT for each channel.

Note that there are two ADFs for each channel, one for each nadir and oblique scan view. In addition, each channel contains a 2-dimension LUT of spectral radiance, one for each detector to allow for differences in the spectral responses of the detectors. However, the temperature-to-radiance LUTs are identical because the spectral responses are the same for each detector and earth view. The radiance in $Wm^{-2}sr^{-1}um^{-1}$ for a specific temperature T(K) can be obtained by quadratic interpolation to the table.

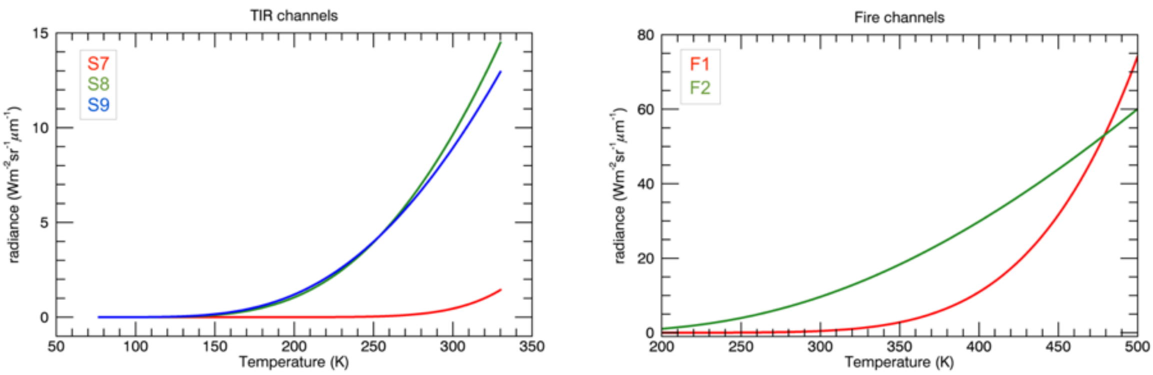

Figure 7: Temperature to radiance LUTs from the Level-1 calibration ADFs for TIR (left) and Fire (right) channels

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5.1.5 Reference NEΔT Model

The SLSTR Level-2 Thermal Infrared (TIR) Noise Data file contains LUTs of NEΔT vs Temperature for each detector and as a function of detector temperature. These tables act as a reference model that allow us to scale the NEΔTs measured at the two internal BBs to the full range of scene temperatures.

Note: The current version of the NEΔT LUTs in the SLSTR Level-2 ADF are based on a theoretical model and pre-launch estimates from the instrument development phase. The pre-launch calibration and in-orbit data show that these estimates were higher than the measured values and a revised model is needed as a reference.

Figure 8 shows the NEΔT model currently included in the SLSTR Level-2 ADF, and the pre-launch calibration measurements.

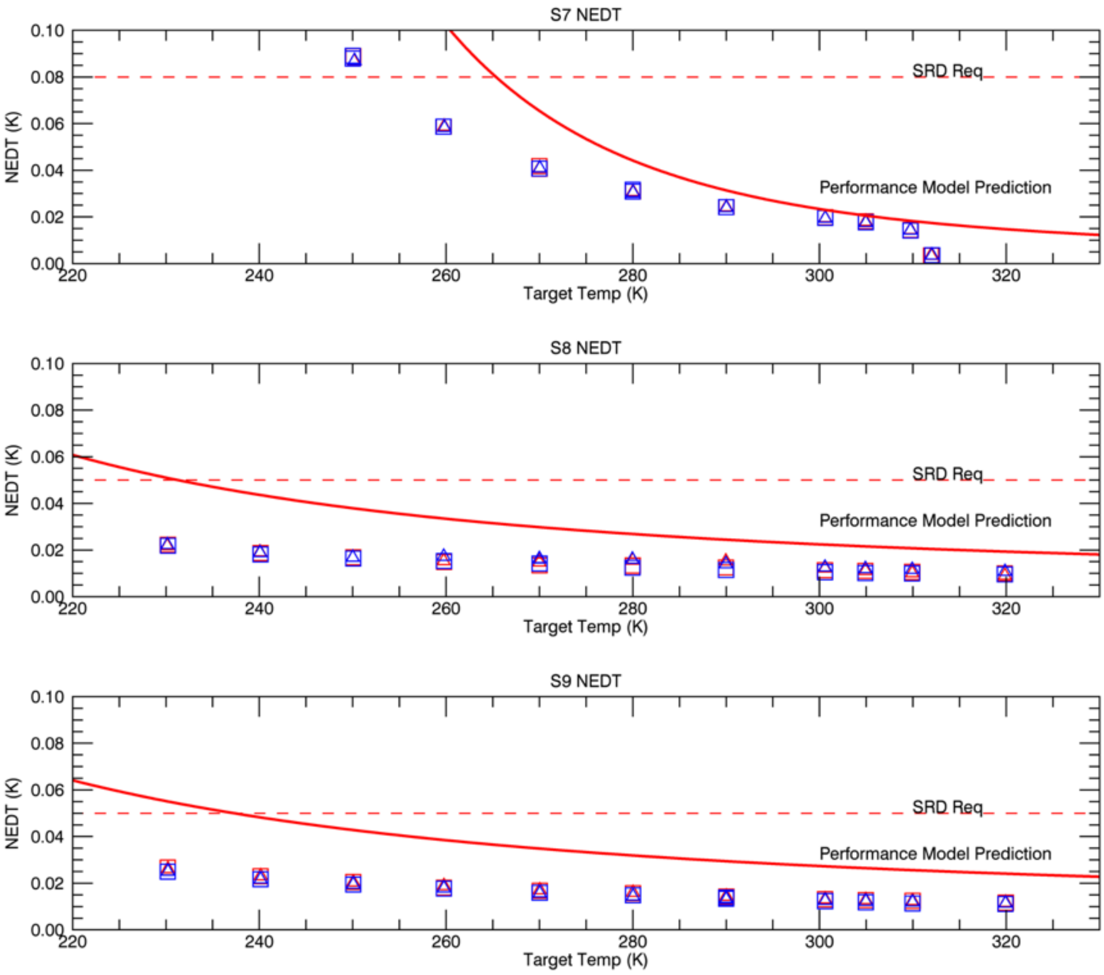

Figure 8: NEΔT versus Temperature for all the TIR channels. (1) NEΔT versus Temperature based on the instrument performance model prediction contained in the SLSTR Level-2 ADF (Red Line). (2) Radiometric noise requirement from the SRD (Dashed red line). (3) Radiometric noise from the blackbody signals as a function of the temperature from the pre-launch calibration tests (Symbols).

5.1.6 Indices Dataset

The Level-1 products contain a NetCDF file of indices which map the gridded pixel detector number in across and along track direction considering 1 km grid for the TIR and Fire channels.

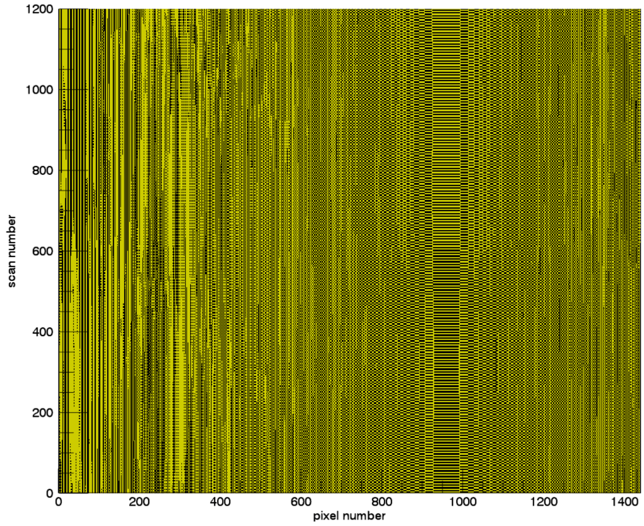

Figure 9: Gridded Level-1 image showing the detector number of each pixel. Yellow shows the pixels associated with detector 1, and in black are the pixels related to detector 2.

5.2 Algorithm Description

The algorithm uses the input files described in the previous section and computes three Level-1 images, one image containing the radiometric calibration uncertainties (systematic effects) and a second image containing the radiometric noise (random) at the pixel level. In addition, the algorithm computes an image of the slope of radiance vs. BT $\left(\frac{\partial L}{\partial T}\right)$ at the pixel level. This image can be used to make the conversion from NE∆T to NE∆L.

5.2.1 Radiometric uncertainties to Level-1 image pixel level

The algorithm calculates the radiometric uncertainty per pixel by interpolation over the Level-1 brightness temperature image (BT_{scene}).

5.2.1.1 Read Data

From the Level-1 product NetCDF files read the following:

a) The Level-1 brightness temperature image, for each channel, and each view

$BT_{scene}[Ni, Nj]$ = <b>_BT_<g><v>.data $[Ni, Nj]$ where Ni, and Nj are the size dimensions of the image

b) The scene brightness temperature range values in the LUT

$BT[N]$ = <b>_quality_<g><v>.scene_temperature.value $[N]$

c) The radiometric uncertainty values in the LUT

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$uBT[N, det]$ = <b>_quality_<g><v>.radiometric_uncertainty.value $[N, det]$

where, N is the number of elements of brightness temperature values and det is the detector number.

5.2.1.2 Create output image

For each channel, we can generate a new image for the uncertainty estimates

$uBT_{scene}[Ni, Nj]$

5.2.1.3 Interpolate to get uncertainty

The scene radiometric uncertainty $uBT_{scene}[i, j]$ is computed by a quadratic interpolation of $uBT[N, det]$ values against $BT[N]$.

We define

$Z = BT_{scene}[i, j]$ as the scene brightness temperature on pixel [i,j]
$Y = uBT[N, det]$ is the radiometric uncertainty equivalent for a range of N brightness temperature values and for each detector given on the Level-1 quality product. However, the radiometric uncertainty is currently the same on both detectors, so we can assume that:
$Y = uBT[N]$
$X = BT[N]$ is the brightness temperature on the Level-1 quality product.

For each pixel [i,j] on the Level-1 image, we define s as the element on the brightness temperature LUT, $X[s]$, that minimizes the function $f = |X[N] - Z[i, j]|$

$$\min(|X[s] - Z[i, j]|) \quad \text{Eq. 4- 1}$$

We define the values:

$$x_0 = X[s - 1] \quad \text{Eq. 4- 2}$$

$$x_1 = X[s] \quad \text{Eq. 4- 3}$$

$$x_2 = X[s + 1] \quad \text{Eq. 4- 4}$$

For each pixel [i,j] on the Level-1 image, the radiometric uncertainty uZ is calculated by a quadratic interpolation defined as:

$$uZ = Y[s - 1]\frac{(Z - x_1) \times (Z - x_2)}{(x_0 - x_1) \times (x_0 - x_2)} + Y[s]\frac{(Z - x_0) \times (Z - x_2)}{(x_1 - x_0) \times (x_1 - x_2)} + Y[s + 1]\frac{(Z - x_0) \times (Z - x_1)}{(x_2 - x_0) \times (x_2 - x_1)} \quad \text{Eq. 4- 5}$$

5.2.1.4 Copy results to image

The result is copied to the uncertainty image such that $uBT_{scene}[i, j] = uZ$.

Figure 10 shows the resulting radiometric uncertainty uBT_{scene} image for channel S8 and for nadir view.

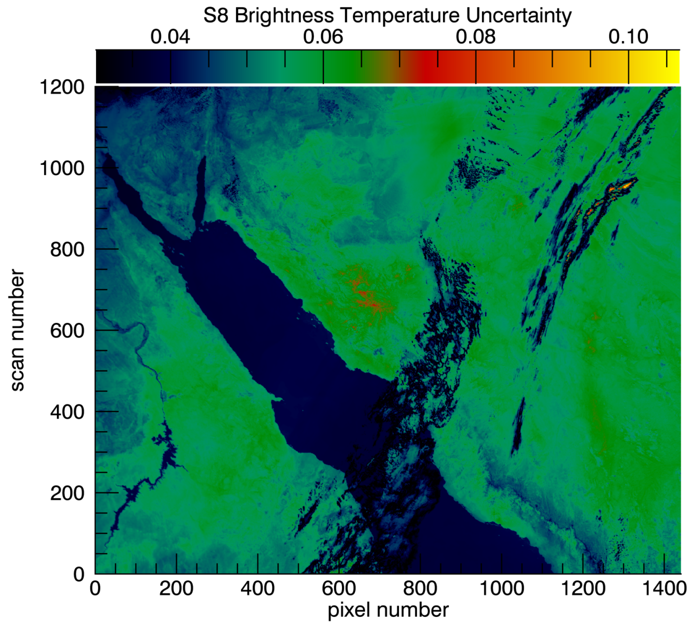

Figure 10 Per pixel radiometric uncertainty estimate from the Level-1 data products for channel S8 and for nadir view

5.2.2 Radiometric Noise

The Level-1 quality data sets contain the signal noise $NE\Delta T_{BB}$ per scan line derived from the two on-board blackbodies. So, the noise estimates are provided for only 2 radiance levels. To determine the signal noise of the Level-1 data products per pixel, we need to interpolate to the full range of scene brightness temperature using the radiometric noise model from the results of the pre-launch calibration.

5.2.2.1 Read input data

From the Level-1 thermal Infrared Quality NetCDF files <b>_BT_quality_<g><v>.nc, for each channel, <b>, and each view, read:

a) the hot and the cold blackbodies temperature

$T_{BBk}[N]$ = T_BB<k>.value$[N]$

b) the corresponding radiometric noise estimates

$NE\Delta T_{BBk}[N, int, det]$ = dT_BB<k>.value $[N, int, det]$

where N is the number of scans, and <k>= 1 or 2 for the hot or the cold blackbody. In addition, the Level-1 Quality data files include the blackbody noise equivalent delta brightness temperature per scan, *N*, and for each detector, *det*, and integrator, *int*

c) Also read in the channel band centre

λ = band_centre.value

From the SLSTR Level-1 TIR ADF file named updated_v3_S3A_SL_CCDB_CHAR_TIR-Calibration-<b>-<v>.nc read:

a) $L1\_BT[N1]$ = TEMPERATURES.value $[N1]$ where *N1* is the total 324 temperature values between 77K and 400K

b) $L1\_rad[N1]$ = RADIANCES.value $[N1, det]$ in $Wm^{-2}sr^{-1}\mu m^{-1}$. For a range of brightness temperature values in the lookup table, the equivalent radiance estimates are the same for both detectors, so $L1\_rad[N1] = L1\_rad[N1{,}0] = L1\_rad[N1{,}1]$

From the SLSTR Level-2 ADF SL_2_<b><v>_AX.nc read the lookup table of detector noise vs. brightness temperature:

a) $L2\_BT[N2]$ = TEMPERATURES.value $[N2]$ where N2 is the total 201 temperature values between 150K and 350K

b) $L2\_NEDT[N2]$ =NEΔT_LUT.value $[v, N2, int, det]$ The file contains the same noise model for every detector, scan view and integrator.

5.2.2.2 Derive Scaling Factor in Radiance Space, *KL*

The response of SLSTR is really a function of the earth scene radiance, so the scaling of the radiometric noise is best performed in terms of radiance, L.

The temperature measured at the blackbodies T_{BBi}, is first converted to radiance L_{BBi} using the temperature-to-radiance LUTs provided. Following the procedure described in Section 5.2.1.3, we define:

- $Z_i = T_{BBi}$ is the granule averaged temperature for the blackbody i.
- $Y = L1\_rad[N]$ is the radiance $Wm^{-2}sr^{-1}\mu m^{-1}$ from the radiance-to-temperature LUT.
- $X = L1\_BT[N]$ is the brightness temperature from the LUT.

$$L_{BBi} = Y[s-1]\frac{(Z-x_1)\times(Z-x_2)}{(x_0-x_1)\times(x_0-x_2)} + Y[s]\frac{(Z-x_0)\times(Z-x_2)}{(x_1-x_0)\times(x_1-x_2)} + Y[s+1]\frac{(Z-x_0)\times(Z-x_1)}{(x_2-x_0)\times(x_2-x_1)} \quad \text{Eq. 4- 6}$$

Where, s is the element on the brightness temperature LUT, $X[s]$, that minimizes the function $f = |X[N] - Z[i,j]|$

$$\min\left(|X[s] - Z[i,j]|\right) \quad \text{Eq. 4- 7}$$

We define the values:

$$x_0 = X[s-1] \quad \text{Eq. 4- 8}$$

$$x_1 = X[s] \quad \text{Eq. 4- 9}$$

$$x_2 = X[s+1] \quad \text{Eq. 4- 10}$$

Figure 11 shows the radiometric noise model from the Level-2 ADF ($NE\Delta L$ vs. L ($Wm^{-2}sr^{-1}um^{-1}$)). We can see that the radiometric noise derived from the BB signals ($ne\Delta l_{BB}$) is lower than the values provided in the auxiliary file. The LUT in the ADF is derived from the instrument performance model provided by industry. This is the 'pre-launch' estimation to give us the shape of the noise curve. However, the actual flight performance is much

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better than the predicted values so, the radiometric noise model needs to be rescaled to the measured blackbody noise provided in the Level-1 data. Applying the quadratic interpolation method defined from Eq. 4-1 to Eq. 4- 5, $NE\Delta L_{BB1}[det]$ and $NE\Delta L_{BB2}[det]$ per granule are estimated for each blackbody averaged radiance (L_{BB1} and L_{BB2}), and for each detector. Together with the radiance per scan for each blackbody (l_{BB1} and l_{BB2}), and the noise per scan $ne\Delta l_{BB1}$ and $ne\Delta l_{BB2}$ for each detector, a scale factor for each detector is defined as:

$$KL[det] = \frac{1}{2N}\left(\frac{\sum_{i=1}^{N} ne\Delta l_{BB1}[i,det]}{NE\Delta L_{BB1}[det]} + \frac{\sum_{i=1}^{N} ne\Delta l_{BB2}[i,det]}{NE\Delta L_{BB2}[det]}\right)$$ Eq. 4- 11

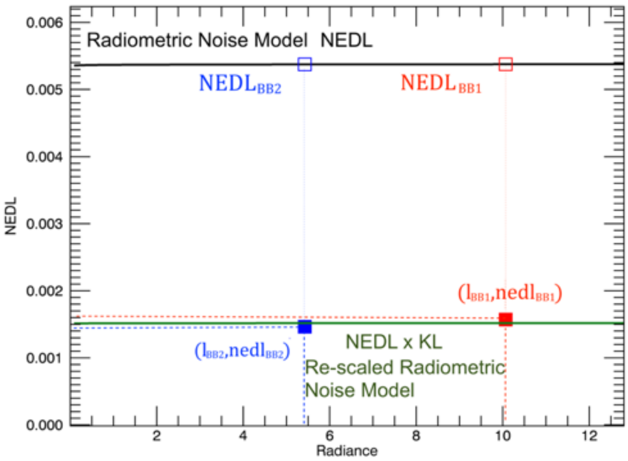

Figure 11: Black curve: Radiometric noise model (NEΔL vs. L(Wm^{-2}sr^{-1}um^{-1})) determined for the instrument performance model. Squares: radiometric noise vs. temperature measured over the cold (blue) and hot (red) blackbodies and averaged over the granule. Green curve: Re-scaled Radiometric noise model (NEΔLx KL vs. L(Wm^{-2}sr^{-1}um^{-1}))

5.2.2.3 Derive new NEΔL values as function of scene radiance

The NEΔL for each detector as a function of scene radiance L$[N]$, is then computed as $L2\_NE\Delta L[N] \times KL[det]$.

5.2.2.4 Convert NEΔL values to NEΔT

We then convert back into NEΔT as a function of BT using

$$NE\Delta T[N,det] = L2\_NE\Delta L[N] \times KL[det] \left(\frac{\partial L}{\partial T}(N)\right)^{-1}$$ *Eq. 4- 12*

Where $\frac{\partial L}{\partial T}(N)$is the slope of radiance vs. BT at the corresponding point in the look-up-table.

This provides new values of NEΔT(N,det) vs BT(N) for each detector element that can be interpolated to the level-1 BT as for the uncertainty estimates.

5.2.2.5 Map NEΔT estimates to Level-1 Image

By knowing which pixel on the Level-1 image is related with which detector, we can interpolate the radiometric noise for each detector on to the Level-1 brightness temperature image.

- $idet$ = indices_<g><v>.detector[i,j] is the detector number of each pixel

- $Z = BT_{scene}[i, j]$ as the scene brightness temperature on pixel [i,j]
- $Y = NE\Delta T[idet, BT]$
- $X = BT$ is the brightness temperature on the noise model LUT.

The radiometric noise $NE\Delta T_{scene}[i, j]$ at the pixel level is determined by interpolation of the new estimates of noise model ($NE\Delta T[idet, BT] \times KT[det]$ vs BT) over each pixel on the Level-1 brightness temperature image, by following equations Eq. 4- 1 to Eq. 4- 5.

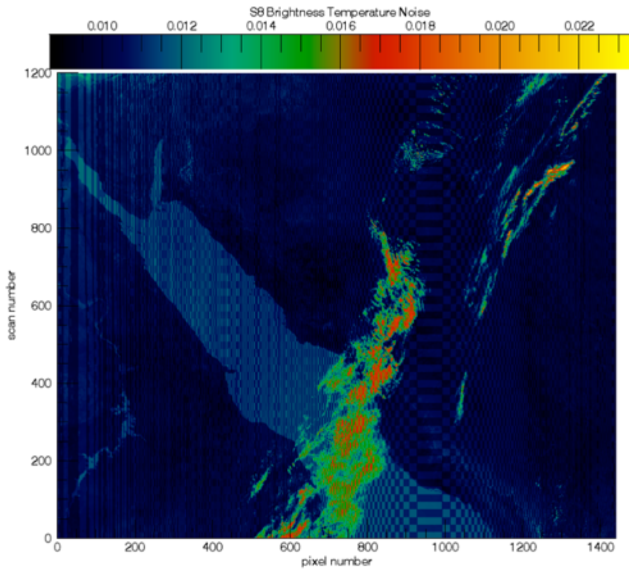

Figure 12 Radiometric noise $NE\Delta T_{scene}$

5.3 Algorithm Output Files

The algorithm provides an output product file in NetCDF format, which is identified as:

<b>_uncertainty_<g><v>.nc

Table 2 shows the CPU processing time for a single channel and for all five TIR/Fire channels processed together for both scan views. In addition, the table contains the output products size in MB.

In order to reduce the output product size, the data are converted to 16-bit signed integer by using the scaling factors and the offsets provided in the attributes of each variable.

The size of one output product containing all the TIR/Fire channels and both views is 86.5 MB. It is only ~15 % of the total size of the original SLSTR Level-1 product.

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Table 2 CPU Processing time and the output product size in MB for the TIR/Fire channels in nadir and oblique views

Channel	Number of Channels	View	Processing Time (CPU)	Product Size (MB)
TIR/Fire	1	Nadir	1.6	10.8
		oblique	1.2	6.5
		nadir & oblique	2.8	17.3
	5	Nadir	7.7	54.0
		oblique	5.0	32.5
		nadir & oblique	13.0	86.5

Every output file contains a set of dimensions, attributes and variables. Table 3 describes the output uncertainty file provided by the Python script.

5.3.1 Global attibutes

The global attributes are defined as follows:

a) '_ncproperties': Version of the NetCDF and the hdf5 libraries used at creation time
b) 'Description': Indicates the channel, the detector array and the scan view
c) 'Source': gives information of the software version used
d) 'References': string containing the ATBD and the IODD documents number
e) 'Product_name': corresponds to the identifier of the input SLSTR Level-1 product package
f) 'LEVEL-1_ADF_Product_name': indicates the identifier to the input SLSTR Level-1 ADF
g) 'L2_ADF_Product_name': indicates the identifier to the input SLSTR Level-2 ADF
h) 'contact': it should contain a EUMETSAT email address
i) 'creation_time': indicates the date and time of when the <b>_uncertainty_<g><v>.nc file was created

5.3.2 Variables and attributes

The output file contains three variables:

1) The brightness temperature uncertainty
2) The noise equivalent brightness temperature
3) The partial derivative of the radiance as a function of temperature $\frac{\partial L}{\partial T}$

Each variable is mapped onto a grid of 1 km resolution. It is a two-dimensional grid defined by the number of rows and columns (across-track and along-track) in the input Level-1 brightness temperature image.

The partial derivative of the radiance as a function of temperature, $\frac{\partial L}{\partial T}$, is provided in the output NetCDF file. This variable allows the user to convert NEΔT to NEΔL

Table 3 Description of the output NetCDF file for TIR channels

```
# dimensions:        2
# Variables:         3
# Global attributes: 9
  There are no unlimited dimensions.

  Dimensions
                 0 Name: along-track    Size:  1200
                 1 Name: across-track   Size:  1500

  Global Atributtes
                 0 _ncproperties:       version=1|netcdflibversion=4.6.1|hdf5libversion=1.10.2
                 1 description:         S3 SLSTR L1 radiometric uncertainty and NEDL. Channel=s8, Array=i, View=nadir
                 2 source:              mapnoiS3.py
                 3 references:          SLSTR-RAL-EUM-TN-003 and SLSTR-RAL-EUM-TN-005
                 4 Product_name:        S3A_SL_1_RBT____20180531T073043_20180531T073343_2018053
                 5 L1_ADF_Product_name: S3A_SL_1_N_S8AX_20160216T000000_20991231T235959_20170324T120000…
                 6 L2_ADF_Product_name: S3A_SL_2_S8N_AX_20000101T000000_20991231T235959_20151214T120000…
                 7 contact              ops@eumetsat.int
                 8 creation_time        Wed Aug 14 10:09:41 2019

  Variables and attributes
                 0 s8_radiometric_uncertainty_in: int16(1500,1200)= int16(across-track,along-track)
                                    0 _FillValue:      -32768
                                    1 Units: K
                                    2 standard_name:   toa brightness temperature uncertainty
                                    3 long_name:       Radiometric uncertainties at the scene BT on the Level-1 image
                                                       per pixel. 1km TIR grid
                                    4 scaling_factor:  1.83082627E-05
                                    5 add_offset:      0.0

                 1 s8_NEDT_in: double(1500,1200)= double(across-track,along-track)
                                    0 _FillValue:      -32768
                                    1 Units: K
                                    2 standard_name:   noise equivalent brightness temperature
                                    3 long_name:       Noise Equivalent brightness temperature at the scene radiance on the
                                                       Level-1 image per pixel. 1km TIR grid
                                    4 scaling_factor:  1.22021700E-06
                                    5 add_offset:      0.0

                 2 s8_dLdT_in: double(1500,1200)= double(across-track,along-track)
                                    0 _FillValue:      -32768
                                    1 Units: mW m^-2 sr^-1 nm^-1 nm^-1 K^-1
                                    2 standard_name:   Partial derivative of the radiance as a function of temperature
                                    3 long_name:       Partial derivative of the radiance as a function of temperature on the
                                                       Level-1 image per pixel. 1km TIR grid
                                    4 scaling_factor:  1.52590218E-05
                                    5 add_offset:      0.0
```

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5.4 Proposed Evolutions

The ADFs were defined long before SLSTR was actually built and they have not been changed since then. In the development of this tool we found several 'features' of the ADF that are either superfluous or missing. We propose a series of modifications on the auxiliary data files:

5.4.1 Changes on the Level-1 ADFs

We proposed to include the temperature and the radiance elements of the temperature-to-radiance lookup table (Section 5.1.4) inside the Thermal Infrared Noise Data file. So, the algorithm would require only one ADF as an input.

5.4.2 Changes on the Level-2 ADFs

1. The Noise Data file now contained in the SLSTR Level-2 ADF is a theoretical model which was defined back to pre-launch calibration. These files will be updated by a new model predicted based on the instrument performance.
2. The dimension of the element NEΔT_LUT is not the same for all the channels. The dimension is [detectors, integrators, Nelem, detector temperature] for channels S8 and S9, and [detectors, Nelem, view] for channels S7 and F1. In addition, there are two independent ADFs for each channel, one for nadir view and one for oblique view, so the dimension related to the scan view is not necessary and should be removed from the NEΔT_LUT element. The values of NEΔT_LUT are also independent of detectors and integrators. For all these reasons, we propose to reduce the dimension of NEΔT_LUT to [Nelem] where Nelem is the number of brightness temperature values in the B_temperature element.
3. The Long_Name value in the element NEΔT_LUT is "S7 nadir single pixel NEΔT estimate LUT" in all ADFs, independently of the channel or the view. The Long_Name value should indicate the channel and the view correctly.

6 Algorithm Description for VIS/SWIR Channels

The estimate of the uncertainties and the radiometric noise at the pixel level is more straightforward for the visible and the SWIR channels than for the TIR and the Fire channels. As in the case of the TIR and Fire channels, the SLSTR Level-1 product package is required as an input in the algorithm. However, the algorithm doesn't need any auxiliary data files or characterization data files.

6.1 Input Files for VIS/SWIR Channels

Figure 13 shows a diagram with the input files necessary for the estimate of the Level-1 uncertainties at the pixel level for the visible and the SWIR channels.

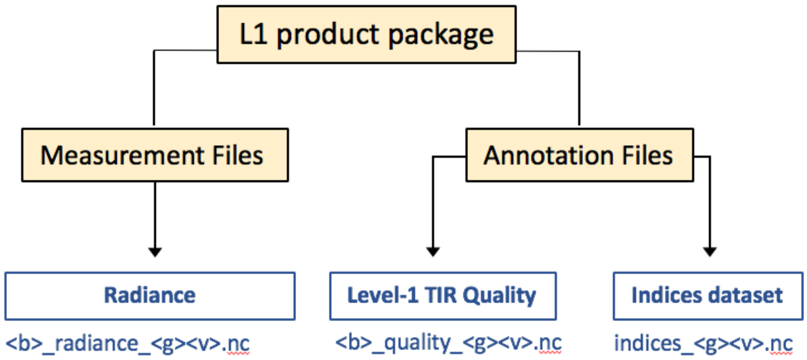

Figure 13 Algorithm input files for the Visible and SWIR Channels.

The sources of information needed to perform the mapping of uncertainty estimates is the SLSTR Level-1 product which is composed of several NetCDF files containing the different measurement and annotation data sets, including:

a) The measurement files include a set of gridded pixel images of radiance in $mWm^{-2}sr^{-1}nm^{-1}$, for each visible channel S1 to S3 and for each SWIR channel S4 to S6.

   The measurement files are named as

   <b>_radiance_<g><v>.nc

   The files are written in NetCDF format and contain a collection of variables and dimensions, sampled at 0.5 km

b) The annotation files contain the Level-1 Visible and Shortwave IR Quality data files. These files contain estimates of detector noise measured at the VISCAL and the blackbodies, as well as radiometric uncertainties calculated in scene radiance and determined during the pre-launch calibration.

   The quality data files are named as

   <b>_quality_<g><v>.nc

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The algorithm also needs information of the gridded pixel detector and scan number in order to assign each detector noise to the corresponding pixel in the gridded image. These data sets are named as

indices_<g><v>

6.1.1 Level-1 radiance data products

The calibrated radiances are mapped onto a rectangular grid of 0.5 km resolution for the visible and the SWIR channels. The measurement datasets are contained in the files:

<b>_radiance_<g><v>.nc

Figure 14 and Figure 15 show a typical S3A SLSTR Level-1 radiance product observed on the 31st May 2018 (orbit 377) by the S2 visible channel and the S5 SWIR channel, in nadir and oblique views. The size of the images is 2880×2400 pixel^2 and 1616×2400 pixel^2 for nadir and oblique view, respectively.

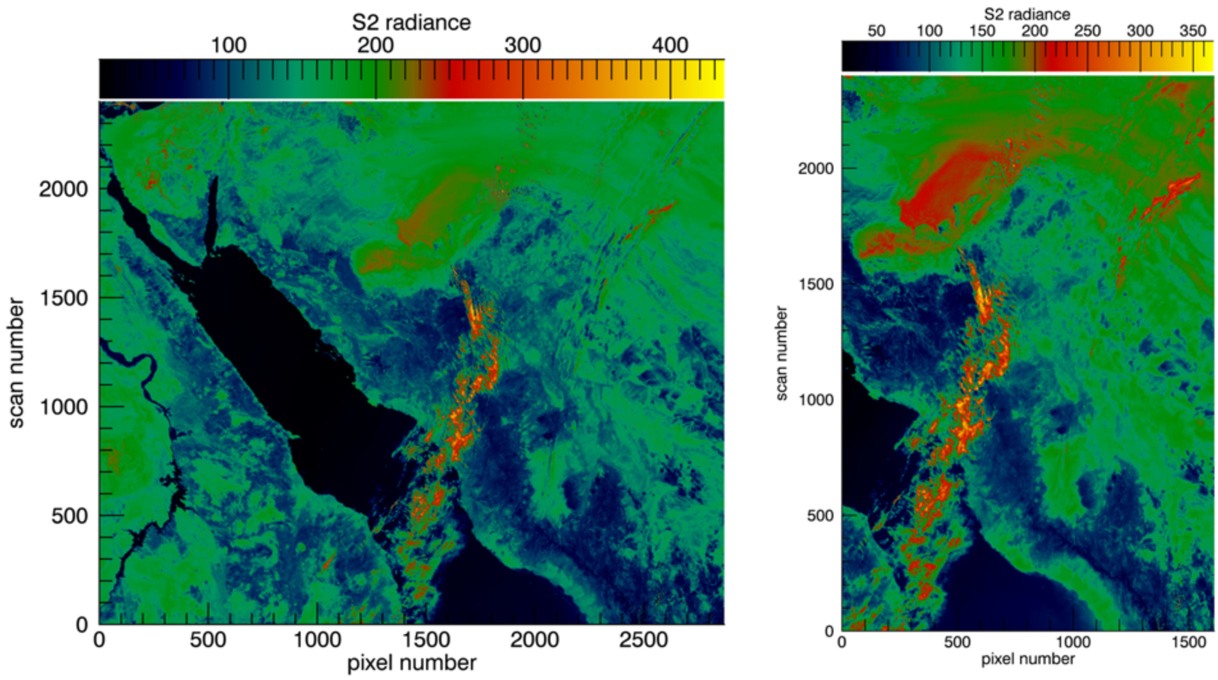

Figure 14 Level-1 Radiance map over Red Sea as observed by the VIS S2 channels in nadir (left) and oblique (right) views.

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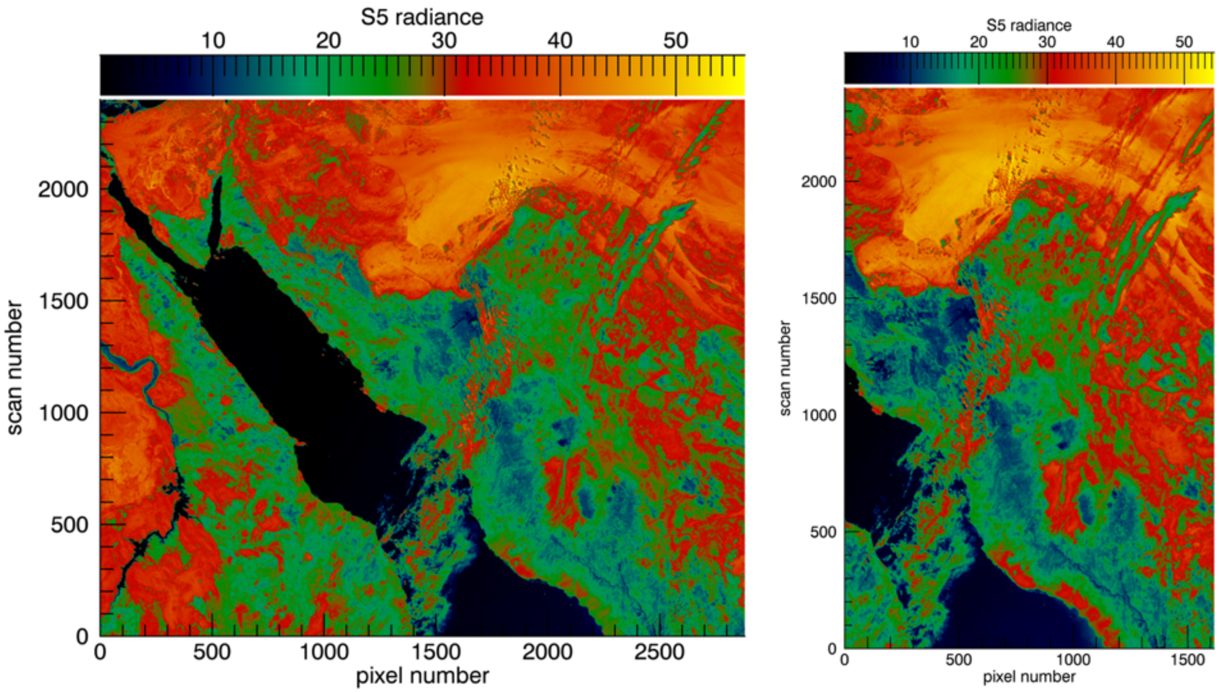

Figure 15 Level-1 Radiance map over Red Sea as observed by the S5 SWIR channel in nadir (left) and oblique (right) views.

6.1.2 Radiometric Uncertainty Estimates

The Level-1 quality products contain a LUT with the scene radiance [mW m^{-2} sr^{-1} nm^{-1}] for the VIS/SWIR channels and the radiometric uncertainty estimates at the equivalent radiance. The LUT is used to derive the radiometric uncertainties at the scene radiance on the Level-1 image per pixel.

The VIS/SWIR channels radiometric uncertainties were derived during the pre-launch calibration by the combined uncertainty budget provided in the calibration report [AD5]. Similar to the TIR channels, the uncertainty cannot be specified for a single value of radiance but it is dependent on the scene radiance.

The maximum scene radiance value in the LUT is limited by the dynamic range of each channel (Table 4), which is defined in the system requirement document [AD6]. For each visible and SWIR channel, the scene radiance to radiometric uncertainty LUT is identical for both views and for all the detectors in the same channel.

Table 4 Dynamic range and maximum scene radiance value in the LUT

Channel	SRD Req. Lmax ($mWm^{-2}sr^{-1}nm^{-1}$)	LUT Lmax ($mWm^{-2}sr^{-1}nm^{-1}$)
S1	585.0	600.0
S2	475.0	500.0
S3	295.0	300.0
S4	113.1	125.0
S5	74.0	75.0
S6	24.3	25.0

The LUT can be used to derive the radiometric uncertainties at the scene radiance on the Level-1 image per pixel. Figure 16 shows the VIS/SWIR channels radiometric calibration uncertainty estimates as a function of the scene radiance.

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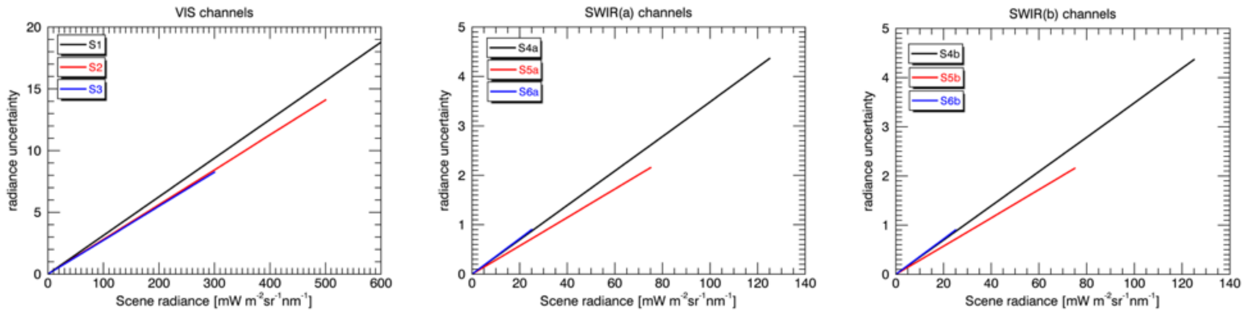

Figure 16 Radiometric uncertainty as a function of scene radiance for visible channels (*left*) and SWIR channels (*centre*: ‘a’ array, *right*: ‘b’ array)

6.1.3 VISCAL radiance and noise

The Level-1 quality data files contain estimates of detector noise measured at the VISCAL, and the ancillary information required to scale these to estimates of radiance noise for each pixel in the visible and the SWIR channels. The VISCAL radiance in units [mW m^{-2} sr^{-1} nm^{-1}], and the VISCAL radiance noise per detector and per scan are provided for channels S1 to S6, from all valid pixels in the VISCAL illumination period. The VISCAL radiance, provided in the Level-1 quality products are estimated as

$$L\_viscal(ch, view, det) = \frac{Reflectance\ factor(ch, view, det) \times solar\ irradiance(ch)}{\pi} \qquad \text{Eq. 5- 1}$$

Where, the $solar\ irradiance(ch)$ is adjusted for earth-to-sun distance seasonally variation
The signal channel noise of the VISCAL signal, $\sigma C_{viscal}(ch, view, t, det)$, is taken as the standard deviation of the detector counts for the VISCAL during the illumination period and is defined by

$$\sigma C_{viscal}(ch, view, t, det) = \left(\frac{1}{M}\sum_{px=m1}^{m2}\frac{1}{N}\sum_{s=n1}^{s=n2}\left(C_{viscal}(ch, view, s, px, t, det) - \bar{C}_{viscal}(ch, view, t, det)\right)^2\right)^{1/2} \qquad \text{Eq. 5- 2}$$

Where, *m1* and *m2* are the start and stop pixels for the view. *M* is the total number of pixels used in the view. *n1* and *n2* are the start and the stop scan of the calibration window.

And the VISCAL radiance noise, *dL_VISCAL*, is calculated as

$$dL\_viscal(ch, view, t, det) = \frac{\sigma C_{viscal}(ch, view, t, det) \times cal\_gain(ch, view, t, det) \times solar\ irradiance(ch)}{\pi} \qquad \text{Eq. 5- 3}$$

The Level-1 quality data files contain the calibration slope for the solar channels, cal_gain, which is estimated as

$$cal\_gain(ch, view, t, det) = \frac{Reflectance\_fator(ch, det) \times gain(ch)}{\bar{C}_{viscal}(ch, view, t, det) - \bar{C}_{BB}(ch, view, t, det)} \qquad \text{Eq. 5- 4}$$

And $gain(ch)$ is the instrument gain setting. For SLSTR the default value is 1.
Note: The signal channel noise of the VISCAL signal taken as the standard deviation of the detector counts for the VISCAL during the illumination period shows strong detector-to-detector variations that are not consistent with the pre-launch values. The discrepancy in the noise estimates is related with the non-uniformity

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of the VISCAL peak surface. So, when the noise is calculated as the standard deviation of the VISCAL counts over the surface peak, the slope of the VISCAL peak contributes to the value giving an over estimation of the noise. Therefore, to derive the noise from the VISCAL signal it is necessary to remove the slope of the VISCAL peak surface first, by fitting a plane to the peak. The processor needs to be modified to obtain a good estimation of the noise at the VISCAL radiance level.

6.1.4 Blackbody radiance and noise

The Level-1 quality data files contain estimates of detector noise equivalent radiances (NE∆L) measured at the cold blackbody.

The blackbody radiance is defined as the average value measured by the cold blackbody over the calibration period (17 PIX10SYNC). For the visible and SWIR channels, the cold blackbody radiance, is equal 0.0, since by definition the blackbodies are assumed to be completely dark.

$$L\_BB(ch, view, t, det) = 0 \qquad \text{Eq. 5- 5}$$

The radiance noise, is estimated from the standard deviation of the detector counts, σC_{BB}, as follows,

The average pixel count from the cold blackbody as a function of channel, scan view, and detector is given as

$$\bar{C}_{BB}(ch, view, t, det) = \frac{1}{M}\sum_{px=m1}^{m2}\frac{1}{N}\sum_{s=s1}^{s2} C(ch, s, px, t, det) \qquad \text{Eq. 5- 6}$$

Where, *m1* and *m2* are the start and stop pixels for the view. *M* is the total number of pixels used in the view. *s1* and *s2* are the start and stop scans of the dark signal calibration window.

The standard deviation of the detector counts is measured over 20 scans, and it is calculated as

$$\sigma C_{BB}(ch, view, t, det) = \left(\frac{1}{M}\sum_{px=m1}^{m2}\frac{1}{N}\sum_{s=s1}^{s=s2}\left(C_{BB}(ch, view, s, px, t, det) - \bar{C}_{BB}(ch, view, t, det)\right)^2\right)^{1/2} \qquad \text{Eq. 5- 7}$$

Finally, the noise radiance measured by the cold blackbody is

$$dL\_BB(ch, view, t, det) = \frac{\sigma C_{BB}(ch, view, t, det) \times cal\_gain(ch, view, t, det) \times solar\ irradiance(ch)}{\pi} \qquad \text{Eq. 5- 8}$$

The calibration slope for the solar channels, cal_gain, is estimated as in Eq. 5- 4

Figure 17 presents the radiance noise for the cold blackbody measured per scan by each detector for channels S2 and S5. The plot clearly shows different detectors measuring different noise radiance.

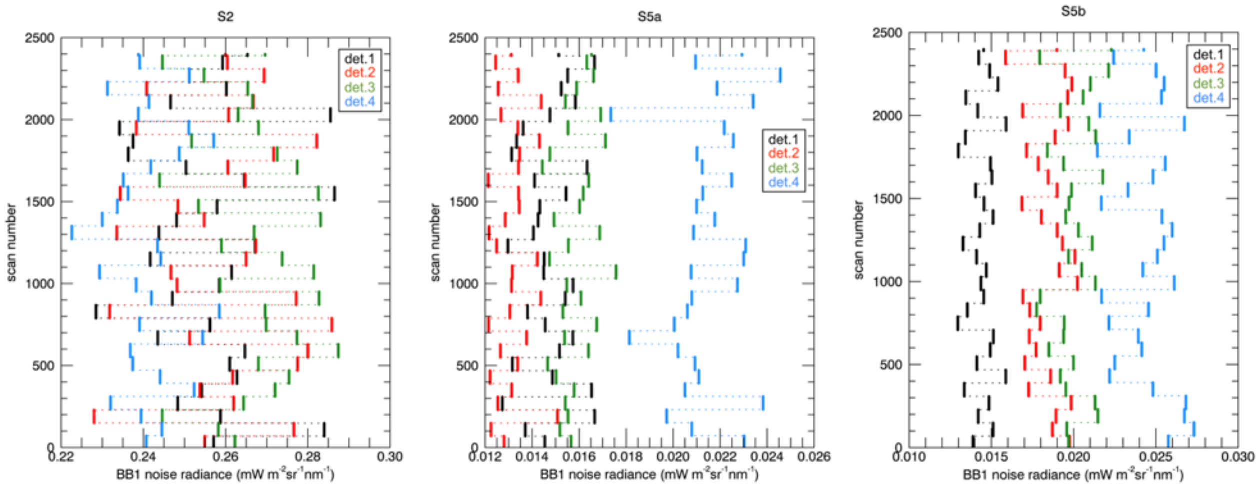

Figure 17 Blackbody radiance noise per scan and per detector determined over the cold blackbody for channels S2, S5a, and S5b

6.1.5 Indices Dataset

The Level-1 products contain a NetCDF file of indices which map the gridded pixel detector number, from detector 1 to detector 4, on the visible and the SWIR Level-1 products (Figure 18) considering 0.5 km grid.

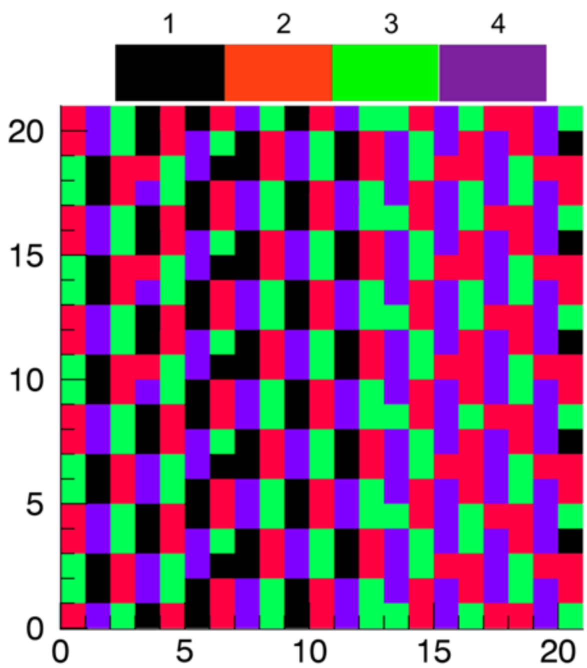

Figure 18 Small sub-region (21 x 21 pixel^2) of the Gridded Level-1 image showing the detector number of each pixel from detector 1 to detector 4

6.2 Algorithm Description

The algorithm uses the input files described in the previous section and computes two Level-1 images for each dataset, one image containing the radiometric calibration uncertainties (systematic effects) and a second image containing the radiometric noise (random) at the pixel level.

6.2.1 Radiometric uncertainties to Level-1 image pixel level

The Level-1 quality products contain a LUT with the radiance (L) for the visible and the SWIR channels, and the radiometric uncertainty estimates (uL) given as NetCDF files. The algorithm uses this LUT in order to calculate the radiometric uncertainty per pixel by interpolation over the Level-1 radiance image (L_{scene}).

6.2.1.1 Read Data

From the Level-1 product NetCDF files read the following:

a) The Level-1 radiance image, for each channel ch, each stripe x, and each view v

$L_{scene}[ch, x, v, Ni, Nj]$ = <b>_radiance_<g><v>.data $[Ni, Nj]$ where Ni, and Nj are the size dimensions of the image

b) The scene radiance range values in the LUT

$L[ch, x, v, N]$ = <b>_quality_<g><v>.scene_radiance.value $[N]$

c) The radiometric uncertainty values in the LUT

$uL[ch, v, N, det]$ = <b>_quality_<g><v>.radiometric_uncertainty.value $[N, det]$

where, det is the detector number. The radiometric uncertainty was calculated for a range of N radiance values, for each detector individually.

6.2.1.2 Create Output Image

For each channel, we can generate a new image for the uncertainty estimates

$uL_{scene}[Ni, Nj]$

6.2.1.3 Interpolate to get uncertainty

Using the Level-1 quality products, we can compute a scene radiometric uncertainty (uL_{scene}) value for each pixel [i,j] on the Level-1 image by a quadratic interpolation of uL values against L.

We define

- $Z = L_{scene}[i, j]$ as the scene radiance on pixel [i,j]
- $Y = uL[N, det]$ is the radiometric uncertainty equivalent for a range of N radiance values, and for each detector given on the Level-1 quality products. However, the radiometric uncertainty is the same on both detectors, so we can define:
  $Y = uL[N]$
- $X = L[N]$ is the radiance on the Level-1 quality products.

For each pixel [i,j] on the Level-1image , we define s as the element on the radiance LUT, $X[s]$, that minimizes the function $f = |X[N] - Z[i, j]|$

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$$\min\left(|X[s] - Z[i,j]|\right) \quad \text{Eq. 5- 9}$$

We define the values:

$$x_0 = X[s-1] \quad \text{Eq. 5- 10}$$

$$x_1 = X[s] \quad \text{Eq. 5- 11}$$

$$x_2 = X[s+1] \quad \text{Eq. 5- 12}$$

For each pixel [i,j], the radiometric uncertainty $uZ = uL_{scene}[i,j]$ is calculated by a quadratic interpolation defined as:

$$uZ = Y[s-1]\frac{(Z-x_1)\times(Z-x_2)}{(x_0-x_1)\times(x_0-x_2)} + Y[s]\frac{(Z-x_0)\times(Z-x_2)}{(x_1-x_0)\times(x_1-x_2)} + Y[s+1]\frac{(Z-x_0)\times(Z-x_1)}{(x_2-x_0)\times(x_2-x_1)} \quad \text{Eq. 5- 13}$$

6.2.1.4 Copy results to image

The result is copied to the uncertainty image such that $uBT_{scene}[i,j] = uZ$.

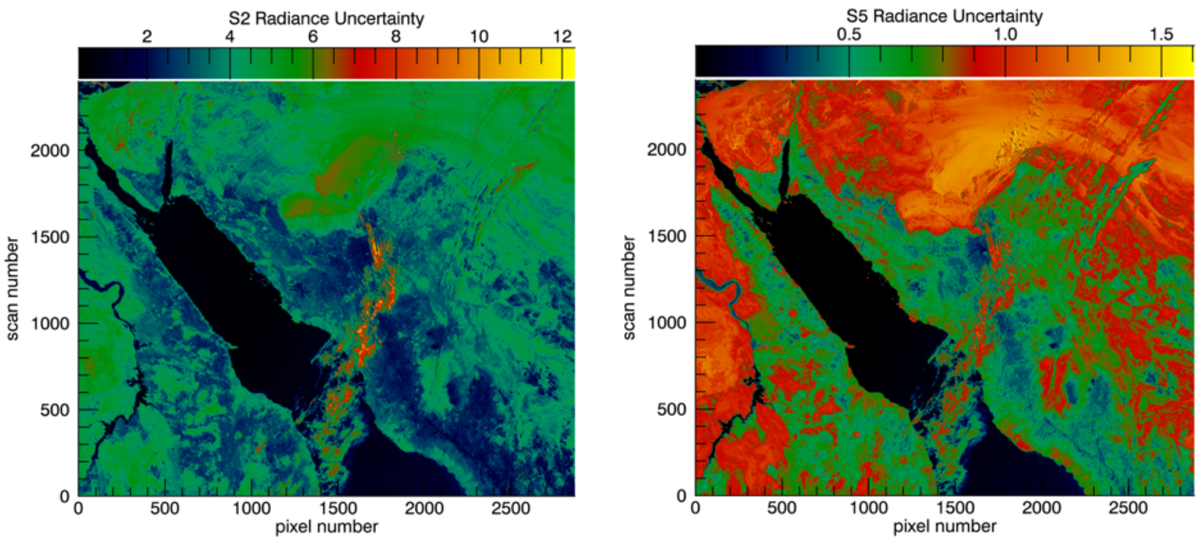

Figure 19: Radiance uncertainty map over Red Sea and Arabian Peninsula for channels S2 (left) and S5 (right)

6.2.2 Radiometric Noise

The total radiometric noise for the visible and the SWIR channels at each pixel level is a contribution of several components: the noise related to the light intensity level (shot noise), and the electronic noise (dark current, amplifier noise, reset noise, digitization) [RP1].

$$\sigma_{total}^2 = \sigma_{shot}^2 + \sigma_{dark}^2 + \sigma_{ampl}^2 + \sigma_{reset}^2 + \sigma_{digit}^2 \quad \text{Eq. 5- 14}$$

At the high-level of quantization of SLSTR (14 bits ADC), the digitization noise is negligible. In addition, the amplifier and the reset noise are insignificant respect to the dark current noise [RP2].

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So, the radiometric noise given in Eq. 5- 14, can be simplified as

$$\sigma_{total}^2 = \sigma_{shot}^2 + \sigma_{dark}^2 \tag{Eq. 5- 15}$$

6.2.2.1 Dark signal noise

From the Level-1 Quality NetCDF files <b>_radiance_quality_<g><v>.nc, for each channel, <b>, each grid <g>, and each view, <v>, read the corresponding radiometric noise estimates

$NE\Delta L_{dark}[N, cyc, det]$ = dL_BB<*k*>.value $[N, cyc, det]$

where N is the number of scans, and *k*= 1 or 2 for the hot or the cold blackbody. In addition, the Level-1 Quality data files include the blackbody noise equivalent delta brightness temperature per scan, *N*, and for each detector, *det*, and integrator, *cyc*

For the derivation of noise per radiance we need to revert back to the raw noise signal using

$$\sigma_{BB}[scan, cyc, det] = \frac{NE\Delta L_{dark}(n, v, cyc, det) \times \pi}{cal\_gain(ch, view, t, det) \times solar\_irradiance(ch)} \tag{Eq. 5- 16}$$

$NE\Delta L_{dark}(n, v, cyc, det)$ = <b>_quality_<*g*><*v*>.dl_bb.value, for channel *b*, detector array *g*, and scan view *v*. This is the blackbody noise radiance measured by each detector in mW m^{-2} sr^{-1} nm^{-1}.

$cal\_gain(cyc, det)$ = <b>_quality_<*g*><*v*>.cal_gain.value $[cyc, det]$ is the calibration slope per cycle and detector in W m^{-2} sr^{-1} units.

$solar\ irradiance(ch)$= <*b*>_quality_<*g*><*v*>.solar_irradiance.value $[det]$ is the solar irradiance all ready earth-to-sun distance corrected in mW m^{-2} sr^{-1} nm^{-1}.

The variation of the detector noise per scan during a whole granule is small compared to the noise levels for all the detectors of the visible and the SWIR channels. Therefore, the detector noise can be estimate as the cold blackbody average noise over the whole granule and both integrators

$$\sigma_{dark}[det] = \frac{1}{2N} \sum_{s=1, cyc=1}^{N,2} \sigma_{BB}[s, cyc, det] \tag{Eq. 5- 17}$$

6.2.2.2 VISCAL signal noise

From the Level-1 Quality NetCDF files <*b*>_radiance_quality_<g><*v*>*.nc*, for each channel, <*b*>, each grid <g>, and each view, <v>, read the corresponding the VISCAL signal noise, σ_{viscal}

The estimate of detector noise is provided at the Level-1 quality products and it is calculated with Eq. 5- 3.

$$\sigma_{viscal}[scan, cyc, det] = \frac{dL\_viscal(n, v, cyc, det) \times \pi}{cal\_gain(ch, view, t, det) \times solar\_irradiance(ch)} \tag{Eq. 5- 18}$$

$dL\_viscal(n, v, cyc, det)$ = <b>_quality_<*g*><*v*>.dl_viscal.value
This is the VISCAL noise radiance measured by each detector in mW m^{-2} sr^{-1} nm^{-1}.

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$cal\_gain(cyc, det) =$ <b>_quality_<*g*><*v*>.cal_gain.value $[cyc, det]$ is the calibration slope per cycle and detector in W m^{-2} sr^{-1}.

$solar\ irradiance(ch)$= <b>_quality_<*g*><*v*>.solar_irradiance.value $[det]$ is the solar irradiance all ready earth-to-sun distance corrected in mW m^{-2} sr^{-1} nm^{-1}.

6.2.2.3 Estimate Shot noise

The shot noise is related with the light intensity level; therefore, it is proportional to the number of photons arriving at the detector. When the detector absorbs a photon, an electron is popped up into the pixel. The accumulated electrons in each pixel is represented by the measured digital counts (DN). As a result, the shot noise measured at the VISCAL unit is proportional to the measured signal as

$$\sigma^2_{shot,viscal} \propto N_{phot,viscal} = K \times (C_{viscal} - C_{dark}) \qquad \text{Eq. 5- 19}$$

where, the C_{viscal} and the C_{dark} are the digital counts measured by the detectors at the VISCAL unit when it is illuminated and obscured, respectively. The Level-1 Quality files don't provide the digital counts at the VISCAL unit, but they contain the parameters needed to derive the signal at the VISCAL.

Following Eq. 5- 1, C_{viscal} can be estimate based on the information provided in the Level-1 Quality files, such as:

$$C_{viscal}(ch, view, t, det) - C_{dark}(ch, view, t, det) = \frac{(L\_viscal(ch, view, t, det) - L\_bb(ch, view, t, det)) \times \pi}{cal\_gain(ch, view, t, cyc, det) \times solar\ irradiance(ch)} \qquad \text{Eq. 5- 20}$$

for each channel ch, stripe x, and scan view v. Since the radiance emitted by the blackbody at visible and SWIR bands is 0 ($L_{bb(ch,view,t,det)} = 0$), then

$$C_{viscal}(ch, view, t, det) - C_{dark}(ch, view, t, det) = \frac{L\_viscal(ch, view, t, det) \times \pi}{cal\_gain(ch, view, t, cyc, det) \times solar\ irradiance(ch)} \qquad \text{Eq. 5- 21}$$

$L_{viscal[det]}$ =<*b*>_quality_<*g*><*v*>.L_viscal.value $[det]$ is the VISCAL radiance measured by each detector in mW m^{-2} sr^{-1} nm^{-1}.

According to Eq. 5- 15, the total noise at the VISCAL is

$$\sigma^2_{viscal} = \sigma^2_{dark} + \sigma^2_{shot,viscal} \qquad \text{Eq. 5- 22}$$

Therefore, we can reduce from equations Eq. 5- 19 and Eq. 5- 22, that

$$K = \frac{\sigma^2_{viscal} - \sigma^2_{dark}}{C_{viscal} - C_{dark}} \qquad \text{Eq. 5- 23}$$

In the other hand, the shot noise measured at the scene level is

$$\sigma^2_{shot,scene} = K \times (C_{scene} - C_{dark}) = K \times \frac{L_{scene}}{cal\_gain} \qquad \text{Eq. 5- 24}$$

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6.2.2.4 Determine total radiometric noise

According to Eq. 5- 15, the total noise at the scene view is

$$\sigma_{scene}^2 = \sigma_{dark}^2 + \sigma_{shot,scene}^2 \quad \text{Eq. 5- 25}$$

Combining equations Eq. 5- 23, Eq. 5- 24, and Eq. 5- 25, the total radiometric noise for the visible and the SWIR channels at each pixel level is

$$\sigma_{scene} = \sqrt{\frac{\sigma_{viscal}^2 - \sigma_{dark}^2}{C_{viscal} - C_{dark}} \times \frac{L}{cal\_gain} + \sigma_{dark}^2} \quad \text{Eq. 5- 26}$$

Where, L is the range of radiance values in mW m^{-2} sr^{-1} nm^{-1}.

6.2.2.5 Convert noise in counts to radiance

The total radiometric noise σ_{scene}, measured by each detector can be estimated as a function of radiance L. The radiance values are limited by the dynamic range of each channel. The range of radiance values are already given in the Level-1 Quality data, in the radiometric uncertainty LUT (see Section 6.1.2)

$L[ch, x, v, N]$ = <b>_quality_<g><v>.scene_radiance.value $[N]$

For each channel, each stripe, each scan view, and each detector, we can develop a radiometric noise model LUT in NetCDF format (Figure 20). The radiometric noise varies as the squared root of signal.

The radiometric noise model should be included on the Level-1 Visible and Shortwave IR Quality data files as a lookup table ($\sigma_{scene}[det]$ vs L). This allows the user to estimate the radiometric noise at the pixel level.

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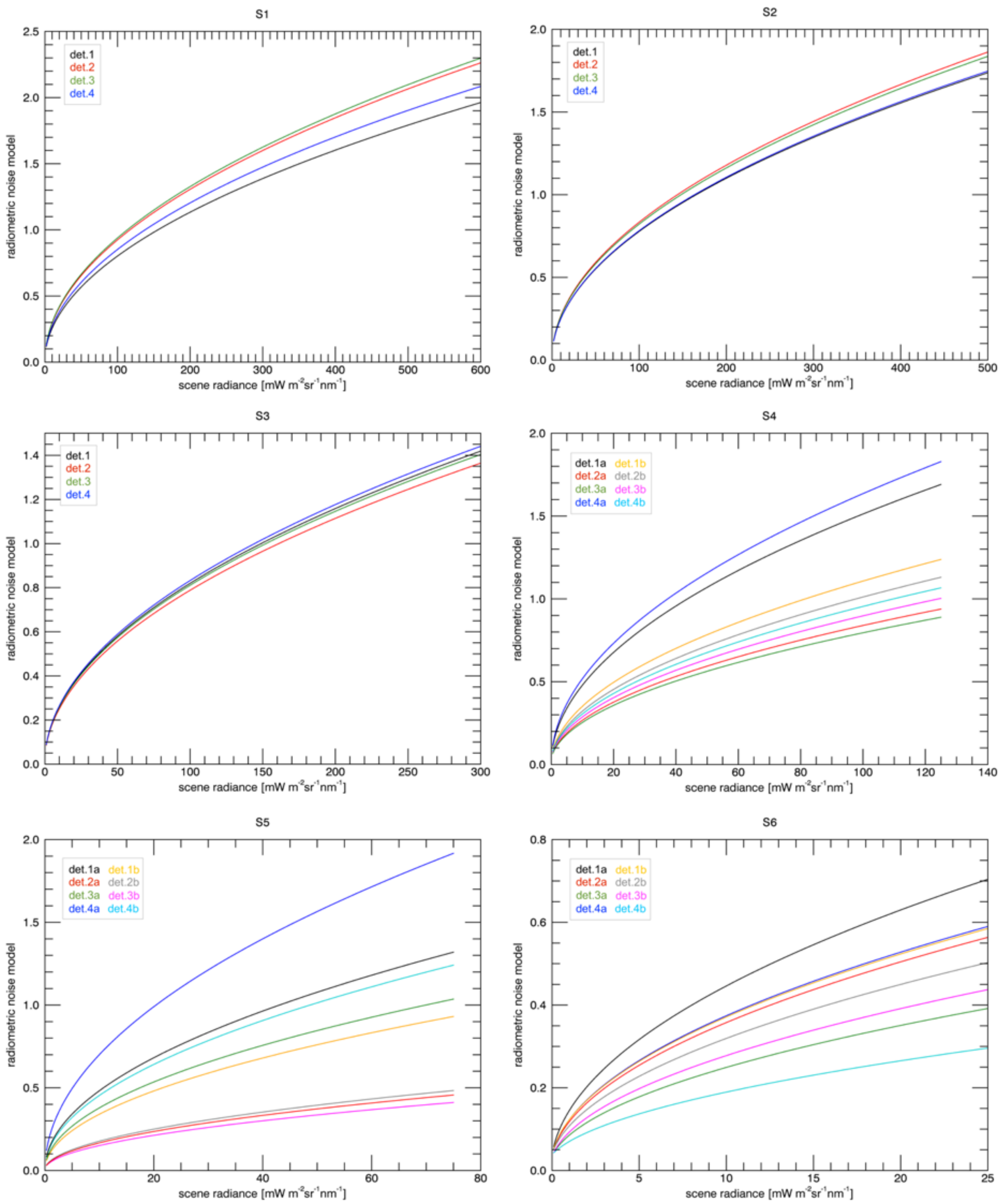

Figure 20 Radiometric Noise model for each channel and each detector in Nadir view.

6.2.3 Map NE∆L to Level-1 image

By knowing which pixel on the Level-1 image is related with which detector, we can interpolate the radiometric noise model (σ_{scene} vs L) for each detector on to the Level-1 radiance image.

- $idet =$ indices_<g><v>.detector[i,j] is the detector number of each pixel
- $Z = L_{scene}[i,j]$ as the scene radiance on pixel [i,j]
- $Y = \sigma_{scene}[idet]$ radiometric uncertainty in the noise model
- $X = L$ is the scene radiance on the noise model LUT.

The radiometric uncertainty for each pixel is then calculated by interpolation following equation Eq. 5- 9 to Eq. 5- 13

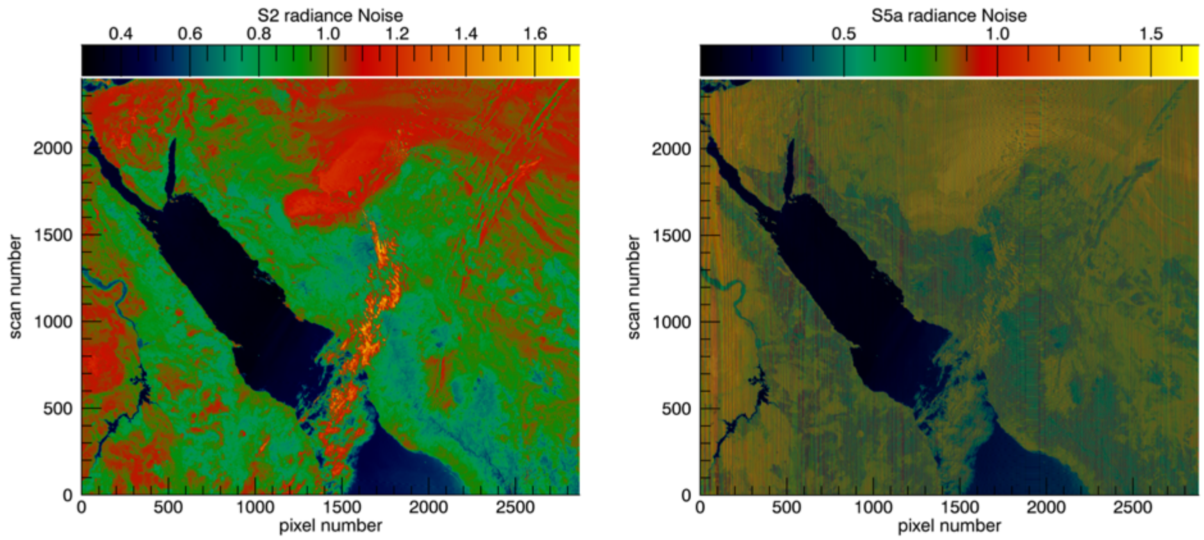

Figure 21: Radiance noise map over Red Sea and Arabian Peninsula for channels S2 (left) and S5 (right)

6.3 Algorithm Output Files

The algorithm provides an output product file in NetCDF format, which is identified as:

<b>_uncertainty_<g><v>.nc

Table 5 shows the CPU processing time for a single channel and for all six VIS/SWIR channels processed together for both scan views. In addition, the table contains the output products size in MB.

The size of the SWIR output products is twice larger than the size of the VIS outputs because, the code provides two NetCDF files, one for each detector array for each SWIR channel.

In order to reduce the output product size, the data are converted to 16-bit signed integer by using the scaling factors and the offsets provided in the attributes of each variable.

The size of one output product containing all the VIS/SWIR channels and both views is 415 MB. It is ~72.9 % of the total size of the original SLSTR Level-1 product

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Table 5 CPU Processing time and the output product size in MB for the VIS and the SWIR channels in nadir and oblique views

Channel	Number of Channels	View	Processing Time (CPU)	Product Size (MB)
VIS	1	Nadir	3.6	28.8
		oblique	2.1	17.3
		nadir & oblique	5.9	92.2
	3	Nadir	11.4	86.4
		oblique	6.9	51.9
		nadir & oblique	18.3	138.3
SWIR	1	Nadir	7.6	57.6
		oblique	4.7	34.5
		nadir & oblique	12.6	92.2
	3	Nadir	20.8	172.8
		oblique	12.7	103.7
		nadir & oblique	33.9	276.6
VIS & SWIR	6	Nadir	32.2	259.3
		oblique	19.8	155.7
		nadir & oblique	52.3	415.0

Every output file contains a set of dimensions, attributes and variables. Table 6 describes the output uncertainty file provided by the Python script.

6.3.1 Global attibutes

The global attributes are defined as follows:

a) '_ncproperties': Version of the NetCDF and the hdf5 libraries used at creation time
b) 'Description': Indicates the channel, the detector array and the scan view
c) 'Source': gives information of the software version used
d) 'References': string containing the ATBD and the IODD documents number
e) 'Product_name': corresponds to the identifier of the input SLSTR Level-1 product package
f) 'contact': it should contain a EUMETSAT email address
g) 'creation_time': indicates the date and time of when the <b>_uncertainty_<g><v>.nc file was created

6.3.2 Variables and attributes

The output file contains two variables:

1) The scene radiance uncertainty
2) The noise equivalent radiance

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Each variable is mapped onto a grid of 0.5 km resolution. It is a two-dimensional grid defined by the number of rows and columns in the input Level-1 radiance image.

Table 6 Description of the output NetCDF file for VIS/SWIR channels

```
# dimensions:        2
# Variables:         2
# Global attributes: 7
  There are no unlimited dimensions.

  Dimensions
                 0 Name: along-track  Size:  2400
                 1 Name: across-track Size:  3000

  Global Atributtes
                 0 _ncproperties:     version=1|netcdflibversion=4.6.1|hdf5libversion=1.10.2
                 1 description:       S3 SLSTR L1 radiometric uncertainty and NEDL. Channel=S5, Array=a, View=nadir
                 2 source:            mapnoiS3.py
                 3 references:        SLSTR-RAL-EUM-TN-003 and SLSTR-RAL-EUM-TN-005
                 4 Product_name:      S3A_SL_1_RBT____20180531T073043_20180531T073343_20180531T093
                 5 contact            ops@eumetsat.int
                 6 creation_time      Wed Aug 14 10:09:41 2019

  Variables and attributes
                 0 s5_radiometric_uncertainty_an: int16(3000,2400)= int16(across-track,along-track)
                                   0 _fillvalue:      32768
                                   1 units:  mW m^-2 sr^-1 nm^-1
                                   2  standard_name:  toa radiance uncertainty.
                                   3 long_name:       Radiometric uncertainties at the scene radiance on the Level-1 image
                                                      per pixel. 0.5km VIS-SWIR grid
                                   4 scaling_factor: 6.10360876E-05
                                   5 add_offset:              0.0

                 1 s5_NEDL_an: int16(3000,2400)= int16(across-track,along-track)
                                   0 _fillvalue:      32768
                                   1 units:  mW m^-2 sr^-1 nm^-1
                                   2 standard_name:   noise equivalent radiance.
                                   3 long_name:       Noise Equivalent radiance at the scene radiance on the Level-1 image
                                                      per pixel. 0.5km VIS-SWIR grid
                                   4 scaling_factor: 5.79842832E-05
                                   5 add_offset:              0.0
```

7 Potential Evolutions

The uncertainty algorithm developed under this contract takes uncertainty information provided in Level-1 products and maps the values for each image pixel.

Random noise effects (NEDT, NEDL) are derived from the on-board blackbody sources and scaled for all scene BTs, radiances via a noise model. Currently the noise model is contained in the Level-2 ADFs which was defined during the Level-2 GPP development based on an early estimation of the noise performance. A modification to the Level-1 ADF is needed to include the noise model based on the actual pre-launch measurements of the SLSTR radiometric noise.

Correlated uncertainties in the Level-1 Quality Auxiliary Data files are derived from the pre-launch calibration and are assumed to be fixed for the mission. No consideration for variations in the flight configuration (instrument temperatures etc..) or instrument drifts are accounted for in the uncertainty estimates.

There are 3 alternative approaches:

1. Update the Level-1 IPF to compute uncertainties directly from the Level-0 data and replacing the existing LUT. Additional parameters are also needed for improving the information in Level-1 products. This would result a moderate change to the Level-1 Quality Auxiliary Data files content. The algorithm could be used to map the uncertainty information for each pixel. This would be the ideal solution since the uncertainty information will be provided directly to the Level-1 users and no further computation is needed.

   This would require an evolution of the Level-1 IPF but is the simplest from a user perspective.

2. Update the Level-1 processor to provide additional parameters in Level-1 Quality Auxiliary Data files to allow uncertainties to be derived as a post-processing. This would be a moderate change to the Level-1 product format and size. Additional parameters include:
   - Blackbody detector counts for each channel and detector
   - Blackbody detector counts noise for each channel and detector
   - Individual thermometer readings for black-bodies (currently baseplate averages are provided)
   - Instrument temperature readings

   The algorithm would need to be modified to compute the uncertainties for each Level-1 product using the uncertainty model.

   A moderate update to the Level-1 IPF is needed since parameters are already computed but not saved in Level-1 Quality Auxiliary Data files.

3. Derive the correlated uncertainties from the outputs of the Level-0 monitoring tools. This would require an evolution to the tools (monitoring and uncertainty tools) to provide the additional functionality. The expected output would be orbital trends and orbital averages of the Level-1 uncertainties. The orbital averages could be an input to the algorithm.

   No update to Level-1 IPF would be needed since all the parameters are generated by the Level-0 monitoring tools. However, several additional steps and tools will be needed to map the derived uncertainties to Level-1 products. This could be difficult to implement in an operational environment since there is no direct link between the Level-0 monitoring and the Level-1 and Level-2 processing chains. Instead this could be seen an interim step to evaluate how Level-1 uncertainties are evolving during the S3 mission, and to explore further the feasibility of implementing options 1 or 2.

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8 Summary

This document presents the algorithm to allow users of SLSTR Level-1 data to derive per pixel uncertainty estimates using the information contained in the Level-1 products, and additional auxiliary data files (ADF).

At this stage, the way the algorithm will be managed is under discussion. The algorithm could either be applied directly by users (by provision of a user tool) or a future upgrade to the IPF processor.

The document describes the datasets required by the algorithm. We propose some modifications of the Level-1 and the Level-2 ADFs required by the algorithm. These ADFs were defined long before SLSTR was actually built and they have not been changed since then. In the development of this algorithm, we found several 'features' of the ADF that are either superfluous or missing. The size of the Level-2 ADF could be reduced by removing the extra dimensions of the Noise Data.

We also propose to include the temperature-to-radiance LUT available in the Level-1 ADF, inside the Noise Data available in the Level-2 ADF. So, all the input datasets required by the algorithm would be available in one set of ADFs.

The derived per-pixel uncertainty information is provided in complementary datasets that are generated. The generated datasets are converted into 16 bits integer to reduce the size of the products. The size of one output product generated for a full SLSTR Level-1 product (all channels and both scan views), is estimate to be 22% smaller than the correspondent input SLSTR Level-1 product.

The CPU processing run time is ~65 with average CPU usage of 45.5 % for a full SLSTR Level-1 product. But, these values are estimate on one particular product, and they might differ from product to product, particularly, when S4 and S7 channels are included in the processing. The processing time of these two channels is subject to cloudiness and saturation, for S4 and S7, respectively.

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