Product User Guide – IASI PCS release 1

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Table of Contents

1 Introduction

1.1 Purpose and Scope

The purpose of this guide is to provide users with detailed information about Release-1 of the Principal Components Scores (PCS) of the Fundamental Data Record (FDR) of the reprocessed Metop-A and B Infrared Atmospheric Sounding Interferometer (IASI) product. The main objective for the IASI measurements is to provide high resolution atmospheric emission spectra to derive temperature, humidity and atmospheric composition profiles with high spectral and vertical resolution and accuracy. Additionally, it is used for the determination of trace gases such as ozone, nitrous oxide, carbon dioxide and methane, as well as land and sea surface temperature, emissivity and cloud properties.

The scope of this document is to inform about the data and method used to derive the PCS, the format the product is available. Several documents listed under reference documents provide complementary information.

This document describes the Metop-A and B PCS IASI Release 1 fundamental data record. The PC scores are in the first step of the level 2 processor and this release consists of a data record generated by the version 6.5.4 2019 of the EUMETSAT operational IASI level 2 processing chain (EUMETSAT, 2018) using the IASI eigenvector files version 1.4 (EUMETSAT, 2010a, 2011).

For this release the reprocessed Metop-A Level 1c (L1c) was used (10.15770/EUM_SEC_CLM_0014 (EUMETSAT, 2019a, 2019b)) until December 2016 and the operational IASI L1c data were used for the rest of the Metop-A period as well as for Metop-B.

This release comprises IASI L1c PCS for IASI onboard Metop-A satellite for the period ranging from the 10 July 2007 until 05 September 2021 and Metop-B from 20 February 2013 to 31 December 2021.

This guide provides:
1. An overview of the specifications of the data record;
2. Background;
3. Technical details on the format and the ordering of the data record, as well as information on the mechanisms to provide feedback.

1.2 Reference documents

Antonelli, P. *et al.* (2004) ‘A principal component noise filter for high spectral resolution infrared measurements’, *Journal of Geophysical Research: Atmospheres*, 109(D23). Available at: https://doi.org/10.1029/2004JD004862.

CEOS/CGMS (2022) ‘Terminology – Climate Monitoring from Space – Joint CEOS/CGMS Working Group’. Available at: https://climatemonitoring.info/home/terminology/ (Accessed: 15 December 2021).

EUMETSAT (2009) ‘IASI PCC FAQ’. Available at: https://www-cdn.eumetsat.int/files/2020-04/pdf_ipcc_faq.pdf (Accessed: 25 October 2022).

EUMETSAT (2010a) ‘EPS Product Validation Report: IASI L1 PCC PPF’. Available at: https://www.eumetsat.int/media/37401.

EUMETSAT (2010b) 'IASI Level 1 PCC Product Format Specification'. Available at: https://www.eumetsat.int/media/6927.

EUMETSAT (2010c) 'IASI Level 1 PCC Product Generation Specification'. Available at: https://www-cdn.eumetsat.int/files/2020-04/pdf_iasi_level1_pcc_prod_gen.pdf.

EUMETSAT (2011) 'EPS Product Validation Report: IASI L1 PCC PPF (Part 2)'. Available at: https://www.eumetsat.int/media/39094.

EUMETSAT (2018) 'IASI L2 PPF v6 : validation report'. Available at: https://www.eumetsat.int/media/45739.

EUMETSAT (2019a) 'Product user guide: IASI level 1c FCDR R 1'. Available at: https://www.eumetsat.int/media/44084.

EUMETSAT (2019b) 'Validation Report – IASI-A Level 1c FCDR release 1'. Available at: https://www.eumetsat.int/media/47452.

EUMETSAT (2020a) 'EUMETSAT data policy'. Available at: https://www.eumetsat.int/media/45173.

EUMETSAT (2020b) 'IASI Level 2: Product Generation Specification'. Available at: https://www.eumetsat.int/media/47444.

EUMETSAT (2020c) 'Validation report of IASI-A and -B climate data record of all sky temperature and humidity profiles'. Available at: https://www.eumetsat.int/media/47744.

EUMETSAT (2022) 'Validation report of IASI-A and -B climate data record of all sky temperature and humidity profiles - extension 2019 to 2018'.

Hilton, F. *et al.* (2012) 'Hyperspectral Earth Observation from IASI: Five Years of Accomplishments', *Bulletin of the American Meteorological Society*, 93(3), pp. 347–370. Available at: https://doi.org/10.1175/BAMS-D-11-00027.1.

WMO, W.M. *et al.* (2011) *GCOS, 154. Systematic Observation Requirements for Satellite-based Products for Climate Supplemental details to the satellite-based component of the Implementation Plan for the Global Observing System for Climate in Support of the UNFCCC : 2011 update*. Geneva: WMO.

1.3 Acronyms and Abbreviations

The table below lists acronyms and abbreviations used in this document:

Acronym	Meaning
AVHRR	Advanced Very High Resolution Radiometer
CDR	Climate Data Record
CEOS	Committee for Earth Observation Satellites
CF	Climate and Forecast
CGMS	Coordination Group for meteorological Satellites
EPS	EUMETSAT Polar System
EUMETSAT	European Organisation for the Exploitation of Meteorological Satellites

FCDR	Fundamental Climate Data Record
FDR	Fundamental Data Record
FoV	Field of View
IASI	Infrared Atmospheric Sounding Interferometer
ICDR	Interim Climate Data Record
IIS	Integrated Imaging Subsystem
L1c	Level 1C
MDR	Measurement Data Records
Metop	Meteorological operational satellite
MDR	Measurement Data Record
PCC	Principle Component Compression
PCR	Principal Component Residuals
PCS	Principal Component Scores
PPF	Product Processing Facility
WMO	World Meteorological Organisation

1.4 Definitions

1.4.1 Principal component scores and reconstruction skills

Operationally, two output products are generated by the IASI L1c Principal Component Compression (PCC) function, namely the product types Principal Component Scores (PCS) and Principal Component Residuals (PCR) respectively. This release consists of the level 1 radiances represented as principal component scores and does not include the PC residuals.

1.4.2 Climate data record definitions

The terminology for Climate Data records have been defined by the joint CEOS/CGMS working group on climate (CEOS/CGMS, 2022).

Fundamental Climate Data Records (**FCDR**s) consist of a consistently-processed time series of uncertainty-quantified sensor observations calibrated to physical units, located in time and space, and of sufficient length and quality to be useful for climate science or applications. FCDRs are typically calibrated radiances, backscatter of active instruments, or radio occultation bending-angles, and include the ancillary data used to calibrate them (WMO *et al.*, 2011).

Climate Data Records (**CDR**s) consist of a consistently processed time series of uncertainty-quantified retrieved values of a geophysical variable or related indicator, located in time and space, and of sufficient length and quality to be useful for climate science or applications.

Interim Climate Data Records (**ICDR**s) are consistently processed times series of uncertainty-quantified estimates of CDR values produced with better timeliness than, but otherwise minimizing differences with, the estimated CDR values.

EUMETSAT produces climate data records (both FCDRs and CDRs) by applying state-of-art data processors, which have advanced significantly during the last decade, to historical and present-day satellite data. EUMETSAT uses in addition the term **Fundamental Data Record** (**FDR**) that is similar to a FCDR but contains only a best possible calibrated single-sensor series. This is often the first step to create multi-sensor cross-calibrated FCDRs. Our climate data records are operationally generated and are routinely checked on quality (***https://www.eumetsat.int/what-we-monitor/climate***)

2 Background

2.1 The IASI Instrument

The Infrared Atmospheric Sounding Interferometer (IASI) is composed of a Fourier transform spectrometer and an associated Integrated Imaging Subsystem (IIS) (Hilton *et al.*, 2012). The Fourier transform spectrometer provides infrared spectra with high spectral resolution between 645 and 2760 cm^{-1} (3.6 µm to 15.5 µm). The IIS consists of a broadband radiometer with a high spatial resolution. However, the IIS information is only used for co-registration with the Advanced Very High Resolution Radiometer (AVHRR). Three IASI instruments are mounted on the Metop satellite series. Metop-A was launched in 2006, Metop-B in 2012 and Metop-C, the last of the series, was launch in 2018.

The IASI instrument observes the Earth up to a viewing angle of 48.3 degrees on either side of the satellite track (Figure 1), thus achieving a nearly daily global coverage. For each view, the instrument analyses an atmospheric cell of about 3.3 degrees x 3.3 degrees, or 50 km x 50 km at nadir. Each cell is analysed simultaneously by a 2 x 2 array of detectors. This geometrical arrangement, together with the step-by-step scanning mode, gives IASI a field of view that can be combined with the other instruments on the platform. The pixel diameter of 12 kilometres at nadir is a trade-off between radiometric performance and likelihood of acquiring measurements in clear-sky, which was originally the prime scope of the mission.

A detailed description of the IASI instrument is given in the IASI Level 2 PGS (EUMETSAT, 2020b).

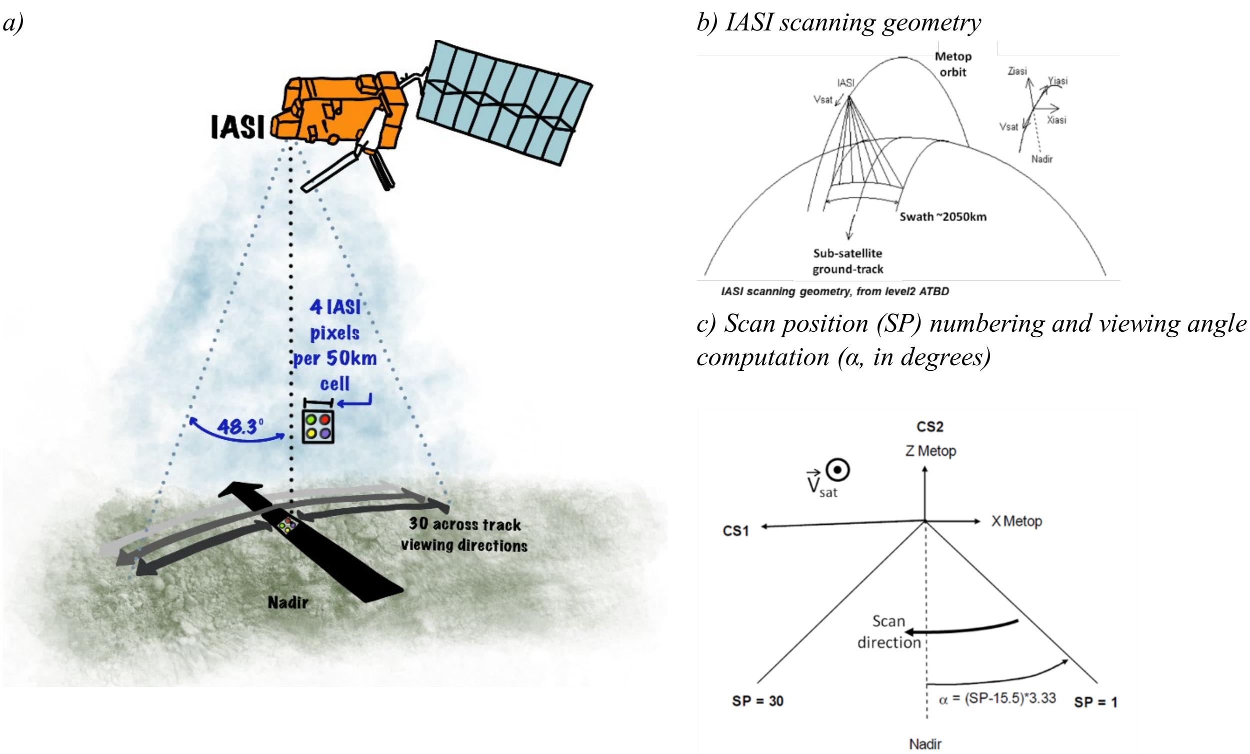

Figure 1: *a) Idealised view of IASI sensing system. b) and c) IASI geometry from level 2* (EUMETSAT, 2020b).

2.2 The level 1C spectrum

IASI level 1c data contain radiance spectra in the unit of $mW/m^2/sr/cm^{-1}$. The data are provided in orbits. Each orbit file contains a similar number of scan lines. The scan starts on the left side with respect to the flight direction of the spacecraft. Each scan line has 30 measuring positions with four pixels each, leading to 120 pixels on each scan line (Figure 2). Each pixel is about 12 km size at nadir.

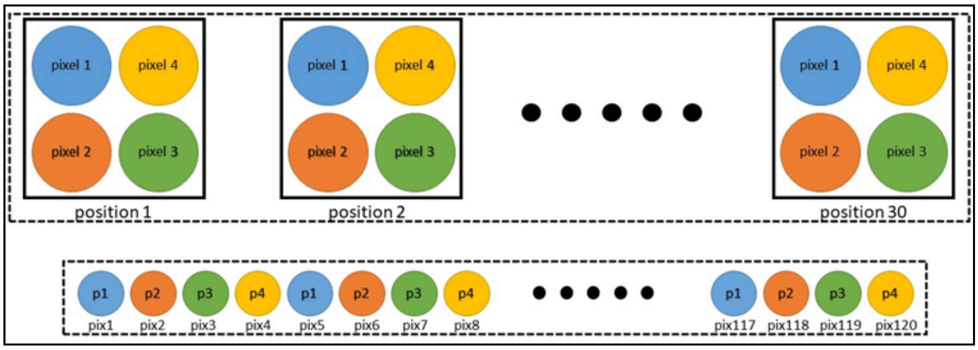

Figure 2: *Idealised view of a pixel for each orbit scan line.*

Figure 3 shows an example of a spectrum for the four individual pixels for one particular scanline and one particular field of view (FoV).

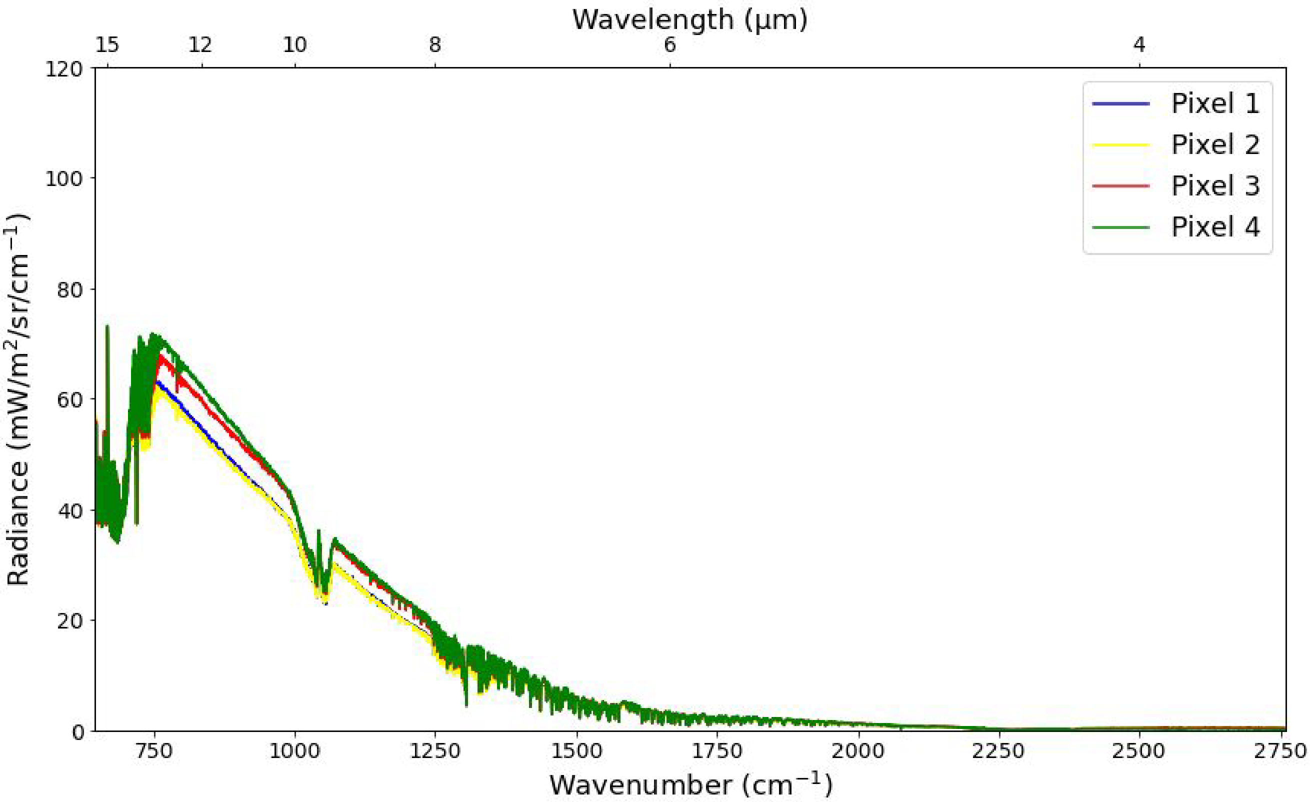

Figure 3: *Example of a IASI spectra for the 4 individual pixels in radiance for IASI onboard Metop-A on the 30th January 2016 starting at 00:56, for the scanline 100 and the FoV=15. (IASI_xxx_1C_M02_20160130005653Z_20160130023852Z_N_O_20160130023752Z.nat).*

2.3 The principal component compression

This section provides a short overview of the IASI PCC operational Product Processing Facility (PPF) functionality that was adapted to generate this FDR.

The purpose of the IASI PCC PPF is to apply principal component compression to IASI L1c radiance spectra. PCC works by representing multidimensional data, like IASI spectra, in a lower dimensional space, which accounts for most of the variance seen in the data. This space is spanned by a truncated set of the eigenvectors of the data covariance matrix. By noise-normalising the spectra prior to the application of the compression technique, the ability to fit the data is enhanced by avoiding giving too much weight to variance caused by noise (Antonelli *et al.*, 2004).

The PCC is applied individually to each of the three IASI spectral bands.

Two output products are generated by the IASI PCC PPF. The two products types are:

- PCS containing a copy of a subset of the Measurement Data Record (MDR) fields (including geolocation, quality flags, satellite and sun angles, etc.) from the input IASI_xxx_1C product as well as the PC scores from which noise-reduced radiances can be reconstructed).
- PCR containing the noise-normalised difference between the original radiances in the IASI_xxx_1C product and the noise-reduced radiances reconstructed from the IASI_PCS_1C product.

This release only contains PCS.

Three eigenvector files (one for each of the three IASI spectral bands) are needed for the application of the PCC. The attribute *Eigenvectorfile* reference the file name of the eigenvector file used for the compression of each of the three spectral bands. The eigenvector files are static auxiliary data files of type IASI_EV1, IASI_EV2 and IASI_EV3 respectively. Their format and the reconstruction steps are specified in the IASI L1C PCC Product Format Specification (EUMETSAT, 2010b).

3 Data record overview

General	Data record name	IASI Principal Component Scores release 1
	Data record digital identifier	10.15770/EUM_SEC_CLM_0084
	Data record short description	Reprocessed PCS IASI data onboard Metop-A and Metop-B satellite
	Record type	Fundamental Data Record (FDR)
	Period covered	**IASI-A**: 10 July 2007 – 5 September 2021 **IASI-B**: 20 February 2013 – 31 December 2022
	Content	Principal components of the IASI L1c (FDR)
	Release date	Q4 2022
	Algorithm version	6.5.4
Instrument	Instrument name	Infrared Atmospheric Sounding Interferometer (IASI)
	Instrument description	The Infrared Atmospheric Sounding Interferometer (IASI) is one of the instruments flying on Metop-A, B and C. The IASI L1c product contains infrared radiance spectra at 0.25 cm^{-1} sampling. The level 1c product has for each sounder pixel 8461 spectral samples covering the range between 645 cm^{-1} and 2760 cm^{-1}. The IASI principal component scores product contains IASI radiance spectra (EUMETSAT, 2010c), compressed by the Principal Component Analysis method.
	Input data	IASI level 1C
	Output data	IASI level 1C principle component scores
	Format	The products are provided in netCDF4
Access	EUMETSAT Data Centre	The data set is available from EUMETSAT Data Centre (https://eoportal.eumetsat.int/)
	Delivery	• ftp push • online pull
Coverage	Spatial	• global • each pixel (IFOV) has a ground resolution of 12 km at nadir
	Temporal	~100 minutes

4 Product definition

4.1 Definition

Principal component compression works by representing multidimensional data, like IASI spectra, in a lower dimensional space, which accounts for most of the variance seen in the data. This space is spanned by a truncated set of the eigenvectors of the data covariance matrix. By noise-normalising the spectra prior to the application of the compression technique, it is ensured that the noise is equally distributed along all directions, leading to an improved signal noise separation.

The coefficients used for the compression are determined by:

1) the training set of IASI L1c spectra, $X \in \mathcal{R}^{mxn}$, where m is the number of channels and n is the number of spectra in the training set,

2) the noise normalisation matrix, $N \in \mathcal{R}^{mxm}$ and

3) the number, s, of eigenvectors to retain.

Let $N^{-1}\bar{x} \in \mathbb{R}^{m}$ and $\mathrm{C} \in \mathbb{R}^{mxm}$ be the mean and covariance of the normalised training dataset $N^{-1}X$ and let $\mathrm{E} \in \mathbb{R}^{mxs}$ be the s most significant eigenvectors of C. The compressed representation (the PC scores), $\mathrm{p} \in \mathbb{R}^{s}$, of a IASI spectrum, $\mathrm{x} \in \mathbb{R}^{m}$, can now be computed as

$$p = E^{T} N^{-1}(x - \bar{x})$$

from which a noise-reduced approximation, $\tilde{x} = NEp + \bar{x} \in \mathbb{R}^{m}$ of x can be reconstructed. For this noise-reduced approximation of the radiances we use the terms "reconstructed" and "noise filtered" radiances synonymously.

The training set used for version 1.4 of the IASI eigenvector files consists of 101902 spectra from the period from December 2007 to August 2010, see (EUMETSAT, 2010a, 2011).

More information and frequently asked questions on the IASI PCS can be found in (EUMETSAT, 2009). Some more information about is content of the NRT files is given in (EUMETSAT, 2010b).

The operational near real time PC compressed IASI L1C products uses a quantisation step of 0.5, such that the disseminated integer values must be scaled by multiplying them with 0.5 to get the PC scores. When reformatting the PC scores to the netcdf format used in this CDR, this scaling has been applied already and the resulting values rounded to nearest integer. This effectively results in a quantisation step of 1 (instead of the original step of 0.5) and therefore a slightly increased quantisation noise.

4.2 IASI L1c spectra

The IASI L1c PCS are divided in three spectral bands listed in Table 1.

Table 1: *Three IASI band limits*

Band	Number of channels	Number range	Wavenumber range
1	1997	0 to 1996	645 to 1144 cm^{-1}
2	3118	1997 to 5115	1144.25 to 1923.75 cm^{-1}
3	3345	5116 to 8460	1924 to 2760 cm^{-1}

The full spectrum is shown in Figure 4 using the original native data (orange) and the reconstructed PCS as input.

An example of code showing how to reconstruct the full spectrum is given in Appendix C.

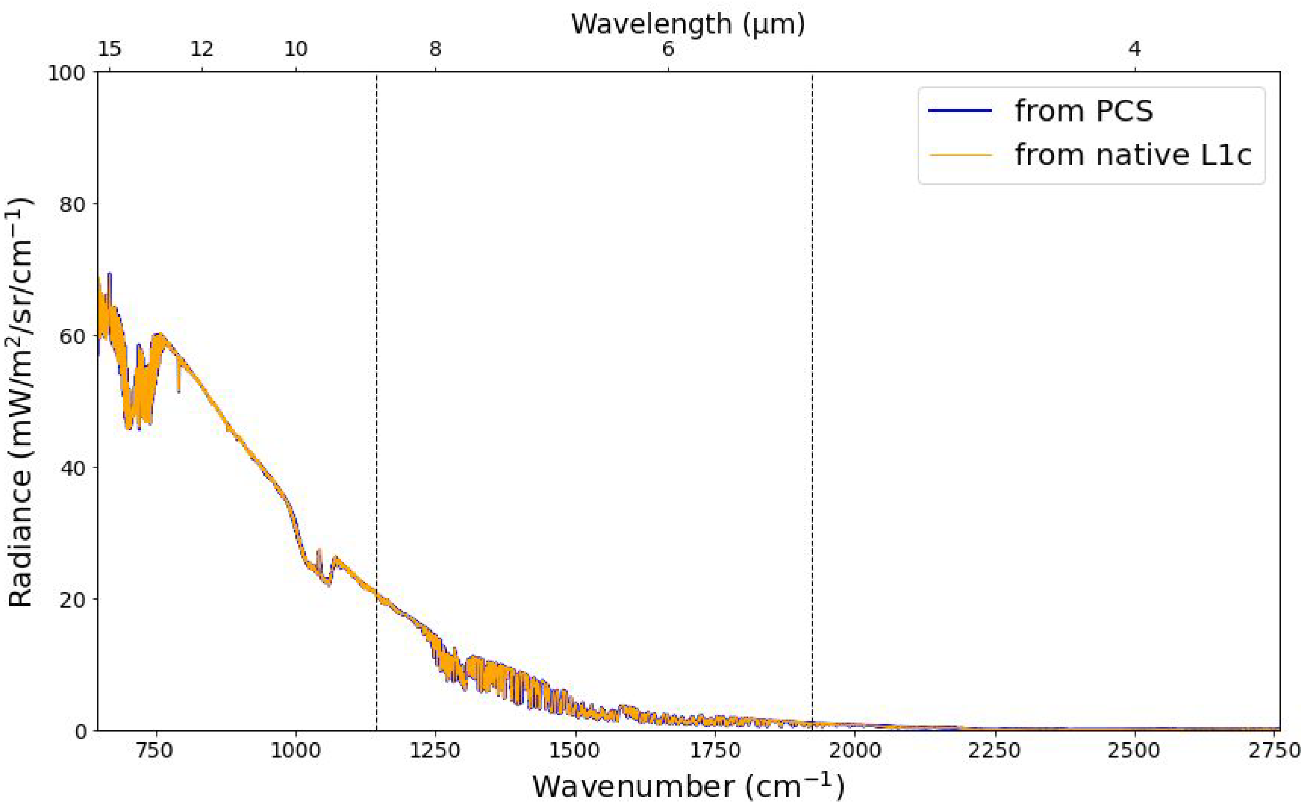

Figure 4: *Example of a IASI L1C spectrum (in orange) and the spectrum reconstructed from its principal components (blue). PCS file W_XX-EUMETSAT-Darmstadt,HYPERSPECT+SOUNDING,METOPA+PCS+IASI_C_EUMP_20160130005653Z_20160130023852Z_eps_r_l2_0100.nc. The spectrum plotted is for the scan line 0 and the 1st pixel of the first field of view. The vertical lines mark the limits of the three bands.*

4.3 Data files content and organisation

4.3.1 Scan line definition

The data are provided in orbits. For this FDR, what is called orbit is in fact a dump (from Svalbard to Svalbard) containing 2 parts of 2 orbits. Each file contains a similar number of scan lines. The scan starts on the left side with respect to the flight direction of the spacecraft. Each scan line has 30 measuring positions with four pixels each, leading to 120 pixels on each scan line (Figure 2). Each pixel is about 12 km size at nadir.

4.3.2 Time

The time of each line can be reconstructed by using the two variables *SensingTime_day* and *SensingTime_msec.* For each line, these two variables provide the sensing date (in days since the 01/01/2000) and the sensing time in the sensing date (in milliseconds) respectively. An example of sensing time computation code is presented in the Table 2.

Table 2: *Example of a python script computing the time for each line.*

```
Compute the time:
import netCDF as nc4
import datetime

def calculate_date_per_line(td,ts):
# Compute the date of each line
#td = SensingTime_day
#ts = SensingTime_msec

    date=[]
    for index in range(0,td.shape[0]):
        r=datetime.timedelta(milliseconds=np.float(ts[index]))
        ref=datetime.datetime(2000, 1, 1,0,0,0,0)+datetime.timedelta(float(td[index]))+r
        date.append(ref)
    return(np.array(date))

f = <IASI_PCS_file>
ncf = nc4.Dataset(f, "r")

timed = ncf. variables['SensingTime_day']
times = ncf. variables['SensingTime_msec']

td    = np.array(timed)
ts    = np.array(times)

date_line = calculate_date_per_line(timed,times)

print(date_line)
```

4.3.3 Variables

The file content is listed in Appendix A. This is a direct copy of the IASI L1c information. All data are in the group L1C. The L1C group contains two subgroups:
- AVHRR containing cluster analysis data of the collocated AVHRR radiances within each IASI footprint,
- PCscores containing the PC scores (divided into 3 subgroups – one for each spectral band)

Additional information such as the time, geolocation and various sun and satellite angles. The land fraction as well as the cloud fraction (derived from collocated AVHRR data) are also provided.

The PC scores are quantised and stored as integers. As the dynamic range of the leading scores in each band is much higher than for the later scores a higher number of bytes are required to represent them. In each band the scores are divided in three parts which are represented with 4, 2 and 1 byte(s) respectively with an associated netCDF variable for each of these three parts.

$N^{-1}(x-\tilde{x})$, where x are the original radiances and $\tilde{x}$ are the reconstructed radiances, is referred to as the noise normalised residual. It's root mean square (within each of the three spectral bands) is stored in the dataset ResidualRMS - high values indicate spectra which are not well represented by the PC scores.

The main quality flag is QFlag. The first three bits (one for each band) reflect the quality of the spectra as reported by the orginal L1C product (GQisFlagQual), whereas bit four to six are based on a comparison of the ResidualRMS, for each band, against a dynamic threshold value as described in the validation report (EUMETSAT, 2010a, 2011). If one of these bits (4 to 6) is set it might be caused by some unusual atmospheric signal which could not be fully captured by the PC scores, but it might also be an indication of increased noise for example due to and undetected spike in the interferogram.

4.4 Temporal coverage

The temporal coverage for IASI onboard Metop-A and –B is given in Table 3.

Table 3: *temporal coverage of the FDR.*

Satellite	Start date	End date
Metop-A	10 July 2007	5 September 2021
Metop-B	20 February 2021	31 December 2021

4.5 Product Format

The Appendix A provides an example of the NetCDF variables and metadata.

The IASI PC score data is available in the Network Common Data Form (NetCDF) format, as a simple conversion from the original native format (not distributed). The file naming of IASI PCS data in NetCDF format follows the standard WMO naming convention.

When possible, the IASI PCS NetCDF variable naming is following the Climate and Forecast (CF) governance standard applied by EUMETSAT to support product development in the frame of the GSICS Data Management Working Group.

4.6 Auxiliary product: the Eigen vectors

The eigenvector files are used for the compression as well as the reconstruction of Level 1C radiances. There is one file for each of the three IASI bands. The three eigenvector file types (IASI_EV1, IASI_EV2 and IASI_EV3) all share the same format. They are HDF5 files containing three Attributes and four Datasets, all belonging to the root group, as detailed in the table Table 8 in Appendix B.

The Eigenvector files are available from the EUMETSAT webpage (www.eumetsat.int), use the search function to find the them.

4.7 File name description

The reprocessed IASI PCS file names follow the WMO file naming convention. An example is given below in Table 4.

***Table 4:** IASI PCS filename description*

Filename convention for reprocessed NetCDF filename	
W_XX-EUMETSAT-Darmstadt,HYPERSPECT+SOUNDING,<SATID>+<PRODUCT>+<INSTRUMENT>_C_<ORIGINATOR>_<DATE>_eps_r_l1_<vvvv>.nc	
Example of a filename	
W_XX-EUMETSAT-Darmstadt,HYPERSPECT+SOUNDING,METOPA+PCS+IASI_C_EUMP_20200101202053Z_20200101220253Z_eps_r_l1_0100.nc	
Description	
<SATID>	Metop-A/B
<PRODUCT>	PCS
<INSTRUMENT>	IASI
<ORIGINATOR>	EUMETSAT (EUMP)
<DATE>	Sensing time start and stop (yyyyMMddhhmmss)
<vvvv>	Version (0100)

4.8 Product generated

The reprocessing was done by EUMETSAT, using IASI L2 PPF version 6.5.4.

5 Validation summary

A specific validation of the IASI Metop-A and B principal component scores (PCS) was not undertaken. As shown in Figure 4, the reconstructed spectra matches the original IASI level 1c spectra very well.
The IASI PCS were used as an auxiliary product used for the generation of the PW3 temperature and profiles (http://doi.org/10.15770/EUM_SEC_CLM_0063). The validation of these profiles showed a very high quality of the CDR (EUMETSAT, 2020c, 2022). We take that CDR validation as an indirect validation of the IASI PCS climate data record release 1.

6 Product ordering

The data are accessible via download from the EUMETSAT Data Store (DS). To access the data from EUMETSAT, you need to register with the EUMETSAT EO-Portal .

6.1 Register with the EUMETSAT and download data

Do this:

1. Register in the EUMETSAT EO-Portal (https://eoportal.eumetsat.int/) by clicking on the New User – Create New Account tab;
2. After finalisation of the registration process, an e-mail is sent to the e-mail address entered in the registration. Click the confirmation link in the e-mail to activate your account;
3. Search for the data in the EUMETSAT Data Store. If the data are no longer available in the DS please contact ops@eumetsat.int for advice.

6.2 Data not available in Data Store

If the data are not available online in the Data Store, please contact ops@eumetsat.int indicating the data record that you want to access including its Digital Object Identifier (DOI) number: *10.15770/EUM_SEC_CLM_0084*.

7 Product support and feedback

For enquiries about the Metop-A and B IASI PCS CDR described in this product user guide, please contact the EUMETSAT User Service Helpdesk by email: *ops@eumetsat.int.*

8 Product referencing

The data record described in this product user guide has a unique DOI that should be used for referencing. The product's filename provides a unique identifier for each product, which is also given in the *id* global attribute

APPENDIX A

Table 5: *List of global attributes.*

Name	Description
title	IASI Principle Component Score CDR
creation_time	File creation date as of yyyy-mm-ddThh:mm:ssZ
creator_email	ops@eumetsat.int
creator_url	www.eumetsat.int
id	DOI: 10.15770/EUM_SEC_CLM_0084
institution	EUMETSAT
source	Operational satellite observation: IASI L1c as input
history	2022-10-27T07:51:28Z netCDF generated from native file
references	DOI: 10.15770/EUM_SEC_CLM_0084
summary	This is the first release of the IASI Principle Component Score (PCS) from METOP. This dataset was reprocessed using the EUMETSAT operational EUMETSAT algorithm v6.5.4 of the EUMETSAT operational IASI level 2 processing chain. Each file contains one full IASI orbit (Svalbard to Svalbard).
comment	For this release data from Metop-A level 1c was used from the release 1 of reprocessed IASI level 1c data (10.15770/EUM_SEC_CLM_0014) and operational level 1c data from Metop-B.
instrument	IASI
platform	MetopA (or MetopB)
orbit_start	First orbit used in file
orbit_end	Last orbit used in file
ParenProduct	IASI L1c file which was the input to this PCS file
processing_level	1C
processing_algorithm_version	6.5.4
product_version	Release 1
Product_name	W_XX-EUMETSAT-Darmstadt,HYPERSPECT+SOUNDING,METOPB+PCS+IASI_C_EUMP_20200101231757Z_20200102005957Z_eps_r_l1_0100.nc
sensing_start_time	yyyy-mm-ddThh:mm:ssZ
sensing_end_time	yyyy-mm-ddThh:mm:ssZ
cdr_platform_start_time	2007-07-10T07:23:58Z (Metop-A) 2013-02-20T03:56:55Z (Metop-B)
cdr_platform_stop_time	2021-09-05T22:20:52Z (Metop-A) 2022-01-01T00:56:53Z (Metop-B)
Processing mode	R
disposition_mode	O
Conventions	CF-1.6
metadata_conventions	Unidata Dataset Discovery v1.0
product_level	1C

Table 6: *IASI PCS netCDF file variables.*

ID	data type	DIM 1	DIM 2	DIM 3	DIM 4	units	Description
/							
CloudFraction	uint8	scan_lines	pixels			%	Cloud fraction in IASI FOV from AVHRR 1B in IASI FOV (from GEUMAvhrr1BCldFrac)
EUMQflag	uint8	scan_lines	pixels				Quality indicator. If the quality is good, it gives the coverage of snow / ice (from GEUMAvhrr1BQual)
EarthSatDistance	uint32	scan_lines					Distance of satellite from Earth center
FLG_SATMAN	uint8	scan_lines					Satellite manoeuvre flag (0=normal, 1=manoeuvre)
InstrumentMode	uint8	scan_lines					161=normal
LandFraction	uint8	scan_lines	pixels			%	Land and coast fraction in IASI pixel from AVHRR 1B (from GEUMAvhrr1BLandFrac)
Latitude	float	scan_lines	pixels			degrees_north	Latitude of ifov
LineNumber	int32	scan_lines					Scanline number in file
Longitude	float	scan_lines	pixels			degrees_east	Longitude of centre of IFOV
QFlag	uint8	scan_lines	pixels				Quality flag. Bit1: Band 1 L1C, Bit2: Band 2 L1C, Bit3: Band 3 L1C, Bit4: Band 1 PCC, Bit5: Band 2 PCC, Bit6: Band 3 PCC
SatAzimuth	float	scan_lines	pixels			degrees	Satellite azimuth angle
SatZenith	float	scan_lines	pixels			degrees	Satellite zenith angle
SensingEndTime_day	uint16	scan_lines				days	UTC-based scanline stop time. Days since 1 January 2000
SensingEndTime_msec	uint32	scan_lines				msec	UTC-based scanline stop time. Milliseconds in day
SensingTime_day	uint16	scan_lines				days	UTC-based scanline start time. Days since 1 January 2000
SensingTime_msec	uint32	scan_lines				msec	UTC-based scanline start time. Milliseconds in day
SunAzimuth	float	scan_lines	pixels			degrees	Sun azimuth angle
SunZenith	float	scan_lines	pixels			degrees	Sun zenith angle
Avhrr/							
RadAnalMean	float	scan_lines	pixels	cluster	AVH_CH	$W/(m^2 \cdot sr)$ and $W/(m^2 \cdot sr \cdot m^{-1})$	Mean AVHRR radiance within the three main radiance analysis clusters
RadAnalStd	float	scan_lines	pixels	cluster	AVH_CH	$W/(m^2 \cdot sr)$ and $W/(m^2 \cdot sr \cdot m^{-1})$	Standard deviation of AVHRR radiance within the three main radiance analysis clusters
RadAnalWgt	float	scan_lines	pixels	cluster			Fraction of IASI FOV covered by the three main AVHRR radiance analysis clusters
T4_mean	float	scan_lines	pixels			$W/(m^2 \cdot sr \cdot m^{-1})$	Overall mean value of AVHRR channel 4
T4_std	float	scan_lines	pixels			$W/(m^2 \cdot sr \cdot m^{-1})$	Standard deviation of AVHRR channel 4
T5_mean	float	scan_lines	pixels			$W/(m^2 \cdot sr \cdot m^{-1})$	Overall mean value of AVHRR channel 5
T5_std	float	scan_lines	pixels			$W/(m^2 \cdot sr \cdot m^{-1})$	Standard deviation of AVHRR channel 5

PCscores/							
Band1/P1	int32	LINE	pixels	B1P1			Band 1 PCScores coded with 4 bytes
Band1/P2	int16	scan_lines	pixels	B1P2			Band 1 PCScores coded with 2 bytes
Band1/P3	int8	scan_lines	pixels	B1P3			Band 1 PCScores coded with 1 byte
Band2/P1	int32	scan_lines	pixels	B2P1			Band 2 PCScores coded with 4 bytes
Band2/P2	int16	scan_lines	pixels	B2P2			Band 2 PCScores coded with 2 bytes
Band2/P3	int8	scan_lines	pixels	B2P3			Band 2 PCScores coded with 1 byte
Band3/P1	int32	scan_lines	pixels	B3P1			Band 3 PCScores coded with 4 bytes
Band3/P2	int16	scan_lines	pixels	B3P2			Band 3 PCScores coded with 2 bytes
Band3/P3	int8	scan_lines	pixels	B3P3			Band 3 PCScores coded with 1 byte
RadianceSum	float	scan_lines	pixels	BND		$W/(m^2 \cdot sr \cdot m^{-1})$	Sum of reconstructed radiances in each band
ResidualRms	float	scan_lines	pixels	BND			Noise normalized residual RMS in each band

Table 7: *Dimension of the variables used.*

ID	Value	Description
scan_lines	variable	IASI scan lines
pixels	120	IASI IFOV number within scan line
cluster	3	AVHRR cluster (3 main clusters)
AVH_CH	6	AVHRR channel number
B1P1	1	Band 1 PC score, stored with 4 bytes
B1P2	41	Band 1 PC score, stored with 2 bytes
B1P3	48	Band 1 PC score, stored with 1 bytes
B2P1	2	Band 2 PC score, stored with 4 bytes
B2P2	61	Band 2 PC score, stored with 2 bytes
B2P3	57	Band 2 PC score, stored with 1 bytes
B3P1	1	Band 3 PC score, stored with 4 bytes
B3P2	44	Band 3 PC score, stored with 2 bytes
B3P3	45	Band 3 PC score, stored with 1 bytes

APPENDIX B

Table 8: *HDF5 objects contained in the eigenvector files.*

Name	Type	Data type	Rank	Dim 1	Dim 2	Description
FirstChannel	Attribute	32-bit integer	0			Channel number (between 1 and 8461) of the first channel of the band.
NbrChannels	Attribute	32-bit integer	0			Number of channels in the band.
NbrEigenvectors	Attribute	32-bit integer	0			Number of eigenvectors included in the file. Can be greater, but not smaller, than the number of PC scores (for the corresponding band) included in the L1 PCS product.
Nedr	Dataset	64-bit floating-point	1	NbrChannels		Random component of the instrument noise assumed for the noise normalisation within the PC compression scheme. [unit: $W/m^2/sr/m^{-1}$]
Mean	Dataset	64-bit floating-point	1	NbrChannels		Noise-normalised radiance means assumed for the PC compression scheme.
Eigenvalues	Dataset	64-bit floating-point	1	NbrEigenvectors		The eigenvalues corresponding to the eigenvector included in the file. **Not used for compression/ reconstruction**.
Eigenvectors	Dataset	64-bit floating-point	2	NbrEigenvectors	NbrChannels	The eigenvectors used for the compression/reconstruction of IASI L1C radiances.

All entities, except Noise, are unit less. The unit of Noise is $W/m^2/sr/m^{-1}$. The eigenvalues are provided for interest only and are not used for compression or reconstruction.

APPENDIX C

In this section we show how to reconstruct the full spectrum from the PCS for one file using the three EV auxiliary files. In this example, the full spectrum containing the 3 bands is reconstructed.

The full spectrum (`full_spectrum`) shape is:
`[number_of_line, number_of_pixels_per line, number_of_channels]`
where `number_of_line` varies from orbit to orbit, `number_of_pixels_per_line = 120`, and `number_of_channels = 8461`.

The program is written in python and uses some generic packages. This is only an example that works on our system but there is not guaranty to work everywhere. The user should get inspired from this and create their own reader.

```
import netCDF4 as nc4
import h5py
import os
import numpy as np
import matplotlib.pyplot as plt

def getscores_from_netcdf_file(band, f):
    print('file to read: ',f, 'for ',band)
    ncf = nc4.Dataset(f, "r")
    p1= ncf.groups['PCscores'][band]['P1']
    p2= ncf.groups['PCscores'][band]['P2']
    p3= ncf.groups['PCscores'][band]['P3']

    return np.concatenate((p1,p2,p3),axis=2)

def get_spectrum_from_band(nc_file, ev_file):

    file_ev = h5py.File(ev_file, "r")

    E = file_ev["/Eigenvectors"][:].T
    Mean = file_ev["/Mean"][:]
    Nedr = file_ev["/Nedr"][:]
    numband = os.path.basename(ev_file)[7:8] # get band (1,2,3) as string from EV filename

    pc_scores = getscores_from_netcdf_file('Band'+numband,nc_file)
    radiance = Nedr * (pc_scores.dot(E.T) + Mean)
    return(radiance)

file = <IASI_PCS_file>

ev_dir=<EV_directory>
ev1_file = 'IASI_EV1_xx_M01_20110125000000Z_xxxxxxxxxxxxxxZ_20110119000104Z_xxxx_xxxxxxxxxx'
ev2_file = 'IASI_EV2_xx_M01_20110125000000Z_xxxxxxxxxxxxxxZ_20110119000104Z_xxxx_xxxxxxxxxx'
ev3_file = 'IASI_EV3_xx_M01_20110125000000Z_xxxxxxxxxxxxxxZ_20110119000104Z_xxxx_xxxxxxxxxx'
evfile_1 = os.path.join(ev_dir, ev1_file)
evfile_2 = os.path.join(ev_dir, ev2_file)
evfile_3 = os.path.join(ev_dir, ev3_file)

spectrum_1 = get_spectrum_from_band(file,  evfile_1)
spectrum_2 = get_spectrum_from_band(file,  evfile_2)
spectrum_3 = get_spectrum_from_band(file,  evfile_3)

full_spectrum = np.concatenate((spectrum_1,spectrum_2,spectrum_3),axis=2)

# example of plot from one spectrum
#-------------------------------------
```

```
ifov = 0 # first pixel on the line
imdr = 0 # first line

# for the radiance *1000*100 to get the correct unit mw/m2/sr/cm-1
plt.plot(full_spectrum[imdr,ifov,:]*1000.*100.,color='orange')

# to get the wave numbers corresponding to each channel
wn = np.linspace(644.75, 2759.75, 8461)
# in wavelength
wl = 1.E4/wn

plt.plot(wn,full_spectrum[0,0,:]*1000.*100.,color='orange')
```