	Summary of activities of NWC SAF clear air team for preparation of MTG-S/IRS L2 from EUMETSAT in CDOP-3	Code: NWC/CDOP3/GEO/AEMET/SCI/RP/NWC-158 Issue: 1.1 Date: 11 March 2022 File: NWC-CDOP3-GEO-AEMET-SCI-RP-sSHAI_ES_NWC-158 Page: 1/46
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Summary of activities of NWC SAF clear air team for preparation of MTG-S/IRS L2 from EUMETSAT in CDOP-3

NWC/CDOP3/GEO/AEMET/SCI/RP/NWC-158, Issue 1, Rev.1


11 March 2022

Prototyping studies sSHAI_ES NWC-158
Applicable to WP2630 in CDOP-3

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DOCUMENT CHANGE RECORD

Version	Date	Pages	Changes
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1.0	21 February 2022	46	First version of the summary of activities of NWC SAF clear air team for preparation of MTG-S/IRS L2 from EUMETSAT central facilities in CDOP-3



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1 INTRODUCTION

The EUMETSAT “Satellite Application Facilities” (SAF) are dedicated centres of excellence for processing satellite data, and form an integral part of the distributed EUMETSAT Application Ground Segment (<http://www.eumetsat.int>).

This documentation is provided by the SAF on Support to Nowcasting and Very Short Range Forecasting, hereafter NWC SAF.

The main objective of NWC SAF is to provide, further develop and maintain software packages to be used for Nowcasting applications of operational meteorological satellite data by National Meteorological Services. More information can be found at the NWC SAF webpage, <http://nwc-saf.eumetsat.int>. This document is applicable to the NWC SAF processing package for geostationary meteorological satellites, NWC/GEO.

1.1 PURPOSE AND SCOPE OF THE DOCUMENT


The purpose of this document is to present a summary of the pioneering activities made by NWC SAF clear air team in CDOP-3 phase related to the preparation for a full and synergetic support of MTG-S/IRS and MTG-I/FCI. In this report it is summarized specifically the activities related to the integration of EUMETSAT MTG-S/IRS L2 products delivered by EUMETCast on local users datacubes in same regions of interest and in the same formats that the used for other NWCSAF product outputs. These consist of netCDF4 files 100% fully CF compliant.

The Working Packages for CDOP-3 was planned in the CDOP-2 and due to the delays in the dates of the launches of MTG satellites and the findings and facts in CDOP-3 some adjustments in the activities has been done. In Figure 1 and taken from [AD.1] the original wording of WP2630 related to MTG-S/IRS L2 activities can be seen. This Working Package can be considered as responsibility of AEMET NWC SAF clear air team. The AEMET clear air team also develops iSHAI product that is the clear air product of the NWC/GEO software package from GEO imager instruments. iSHAI (**i**maging **S**atellite **H**umidity **A**nd **I**nstability) is, since version 2016, the name of the clear air product of the NWC/GEO software package from GEO imager instrument.

Since EUMETSAT has not provided MTG-S/IRS L2 test files, the main focus in this document are the activities made by the NWCSAF clear air team to continue developing software to remap IRS L1 and L2 files to MTG-I/FCI grid using as proxy other satellite data and products. Also, some tests have been made to remap from other satellite to a proxy of IRS dwell file. It is described the path followed from the early attempts to the latest version. Some of these developments have been used now with the AEMET PGE00* tools (using RTTOV-13.0 version; see [RD.1] and [RD.2]) to generate the first scientifically correct synthetic MTG-S/IRS and MTG-I/FCI L1 data using a local NWP model complemented with ECMWF model.

All these activities have been made as preparation for a future full and synergistic use of MTG-S/IRS and MTG-I/FCI data and products from the METEOSAT Third Generation (MTG) on the NWCSAF/GEO software packages.

In the case of the MTG-I/FCI, NWCSAF GEO software package for MTG-I/FCI Day-1 will be a continuation of the current NWCSAF GEO package with almost the same products (cloud mask, iSHAI, etc.) but with improved performances due to the use of the new FCI channels and improved characteristic of FCI. After the delivering of iSHAI software version 2021 and before end CDOP-3, it has been considered the best time to write this report because also it could be used as an introduction and a basis for planning of some activities included in next CDOP-4 phase.

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In the case of the MTG-S/IRS hyperspectral instrument one optional and independent IRS NWCSAF GEO software package for MTG-S/IRS Day-2 will be developed. The idea is that the IRS NWCSAF/GEO software package be operated in coordination with FCI NWCSAF/GEO software package; in order to share as much as possible the infrastructure and allowing the synergetic exploitation of FCI and IRS data and products by the users. Something that is important to note is that one of the main purposes of sSHAI_ES is to remap EUMETSAT Secretariat IRS L2 file on the same NWCSAF users' region in FCI IR grid than IRS L1, FCI L1 and FCI L2 files to build local users data cubes.

The IRS NWCSAF/GEO software package will provide three main services or products to users:

Quick-IRS L1: support of the MTG-S/IRS L1 activities for local generation simple products of image type and for the use IRS L1 as input for local generation of NWC SAF or user's products. As example they could be generated:

- MTG-S/IRS RGB images
- Generation of MTG-S/IRS observed radiances
- Normalized IRS-L1 channels in spectral region such as CO₂ or WV branches representing the state of the atmosphere at several layers.
- Simple operations with MTG-S/IRS L1 fields as differences or regressions between several IRS channels.
- Blending products generated with the combination of FCI and IRS data.

Thus, users could made the automatic generation of IRS L1 imagery related products or to use them for locally generation of NWC SAF or users products. The activities related to the preparation of Quick-IRS L1 are the main objective of [RD.2] Scientific Report.

sSHAI ES: support of the MTG-S/IRS L2 files generated centrally by EUMETSAT Secretariat (ES) on EUMETSAT headquarters for the IRS full disk. These IRS L2 files will be distributed to the users using EUMECast (satellite or terrestrial) on dwell by dwell files; each dwell covering a region of 160x160 pixels. sSHAI_ES will made the reading, conversion, calculation of parameters, concatenation and remapping from the needed dwell files to files on NWCSAF regions. Thus, sSHAI_ES MTG-S/IRS L2 fields could be used directly by users in combination with the ones L1 and L2 fields from FCI or IRS for the same regions. As an example, the comparison of instability indices or precipitable water fields from MTG-I/FCI, MTG-S/IRS and NWP. The activities related to the preparation of sSHAI_ES are the main objective of this Scientific Report.


sSHAI: development of product executed locally by the users. Local generation of NWCSAF MTG-S/IRS L2 product using algorithms with light CPU demand.

As can be seen in the name of the products prefix “i” indicates generated with input data from one GEO imager instrument and “s” prefix will indicate generated with input data from MTG-S/IRS sounder instrument.

In all the IRS services and products it will also be made the concatenation and reprojection from the “dwell” files disseminated by EUMETSAT to users regions of interest on FCI IR grid on resolution of 2x2 boxes ($\approx 4 \times 4$ km spatial resolution on nadir) or 1x1 boxes depending on user's choices.

There are also some remarkable points in the activities described in this report:


- a) Some of the tests have been made based on AEMET PGE00* tools. The PGE00* tools use 4D interpolated NWP profiles to get synthetic data for imager (MSG, GOES-R, MTG-I/FCI) or sounder (MTG-S/IRS and IASI) instruments on clear and cloudy conditions; see [RD.1] and

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[RD.2]. The use of the AEMET PGE00* involves as first step the 4D interpolation from GRIB files of some NWP models to get vertical, spatial and temporally collocated NWP and satellite. This 4D interpolated profiles and data used as input to PGE00* tools can also be written on binary files. Thus, together with the synthetic data also the 4D data cube used for the generation of the synthetic data is available and it can be used as “truth” for training, performance assessments and validation in the developments. In this Report it has been used as proxy of future EUMETSAT Secretariat L2 products.

b) Also these binary files can be converted to netCDF files to be used on meteorological tools.
c) It has been used McIDAS-V tool as main visualization tool and proxy of future user needs and tools. The use of McIDAS-V tool as main visualization tool of this report allows to manage interactively and at the same time the synthetic IRS and FCI data cubes together with the 4D NWP data cubes. McIDAS-V can be considered as proxy of future user needs and tools for IRS use in nowcasting.


Some of the results and Figures described in this Scientific Report have been shown in several workshops or communicate to EUMETSAT on private discussions. It will be indicated in each chapter.

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1.2 DEFINITIONS, ACRONYMS AND ABBREVIATIONS

Please refer to the “Nowcasting SAF Glossary” document in the NWC SAF web for a wider glossary and a complete list of acronyms for the NWC SAF project.


ABI	Advanced Baseline Imager
AEMET	Agencia Estatal de Meteorología Meteorology State Agency (Spain)
AHI	Advanced Himawari Imager
ASCII	American Standard Code for Information and Interchange
ATBD	Algorithm Theoretical Basis Document
BL	Precipitable water in low layer ($P_{\text{sfc}} - 850 \text{ hPa}$)
BT	Brightness Temperature
CDOP (CDOP-1)	Continuous Development and Operations Phase (1)
CDOP-2	Continuous Development and Operations Phase 2
CDOP-3	Continuous Development and Operations Phase 3
CF	NetCDF Climate and Forecast (CF) Metadata Conventions
CIMSS	Cooperative Institute for Meteorological Satellite Studies (USA)
CMa	Cloud Mask
COTS	Commercial-Off-The-Shelf
CPU	Central Processor Unit
DEM	Digital Elevation Model
ECMWF	European Centre for Medium-range Weather Forecasts
EOF	Empirical Orthogonal Function
EUMETSAT	European Organisation for the Exploitation of Meteorological Satellites
FCI	Flexible Combined Imager (MTG)
FG	First Guess
FOV	Field Of View
FOR	Field Of Regard
GEO	Geostationary Satellites
GEO-CMa	GEO Cloud Mask and Cloud Amount

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GEO-iSHAI	GEO imaging Satellite Humidity And Instability
GRIB	Gridded Information in Binary Form
HDF5	Hierarchical Data format version 5
HL	Precipitable water in High Layer (500 – 0 hPa)
hPa	Hecto Pascal
HRIT	High Rate Image Transmission
IDL	Interactive Data Language
IR	InfraRed
IREMIS	InfraRed Emissivity
IRS	Infrared Sounder (MTG)
iSHAI	imaging Satellite Humidity And Instability
K	Kelvin
KI	K-Index
km	kilometre
LI	Lifted Index
LPW	Layer Precipitable Water
LST	Land Surface Temperature
MARS	ECMWF Meteorological Archive and Retrieval Facility
McIDAS	Man Computer Interactive Data Access System
ML	Precipitable water in Medium Layer (850 – 500 hPa)
MSG	Meteosat Second Generation
MTG	Meteosat Third Generation
MTG-I/FCI	Meteosat Third Generation Flexible Combined Imager
MTG-S/IRS	Meteosat Third Generation Infra Red Sounder
netCDF	Network Common Data Form
NRT	Near Real Time
NWC	Nowcasting
NWC/GEO	Geostationary part of the Nowcasting SAF
NWCLIB	Nowcasting Library

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NWCSAF	Nowcasting SAF
NWP	Numerical Weather Prediction
NWP SAF	SAF for Numerical Weather Prediction
LPW	Layer Precipitable Water
PGE	Product Generation Element PGE01 Cloud Mask (GEO-CMa) Product Generator PGE13 SEVIRI Physical Retrieval (SPhR) Product Generator
PW	Precipitable Water
RTM	Radiative Transfer Model
RTTOV	Radiative Transfer for TOVs
SAF	Satellite Application Facility
SEVIRI	Spinning Enhanced Visible InfraRed Imager
SG	Steering Group
SHAI	Satellite Humidity And Instability
SHW	Showalter Index
SKT	Skin Temperature
SST	Sea Surface Temperature
SW	Software
TOZ	Total ozone
TPW	Total Precipitable Water
TM	Task Manager
UM	User Manual
VR	Validation Report
VSA	Visiting Scientist Activities
WV	Water Vapour Channel

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1.3 REFERENCES

1.3.1 NWC SAF Applicable Documents

The following documents, of the exact issue shown, form part of this document to the extent specified herein. Applicable documents are those referenced in the Contract or approved by the Approval Authority. They are referenced in this document in the form [AD.X]

For versioned references, subsequent amendments to, or revisions of, any of these publications do not apply. For unversioned references, the current edition of the document referred applies.

Current documentation can be found at the NWC SAF Helpdesk web: <http://nwc-saf.eumetsat.int>.


Ref.	Title	Code	Vers
[AD.1]	Proposal for the Third Continuous Development and Operations Phase (CDOP-3) March 2017-February 2022	NWC SAF: CDOP-3 proposal	1.0
[AD.2]	Project Plan for the NWCSAF CDOP3 phase	NWC/CDOP3/SAF/AEMET/MGT/PP	1.6

Table 1: List of Applicable Documents

1.3.2 Reference Documents


The reference documents contain useful information related to the subject of the project. These reference documents complement the applicable ones, and can be looked up to enhance the information included in this document if it is desired. They are referenced in this document in the form [RD.X]

For dated references, subsequent amendments to, or revisions of, any of these publications do not apply. For undated references, the current edition of the document referred applies.

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Ref.	Title	Code	Vers	Date
[RD.1]	Summary of activities of NWC SAF clear air team for preparation of MTG-I/FCI in CDOP-3	NWC/CDOP3/GEO/AEMET/SCI/RP/synthetic_FCI	1.0	31/01/22
[RD.2]	Summary of activities of NWC SAF clear air team for preparation of MTG-S/IRS L1 in CDOP-3	NWC/CDOP3/GEO/AEMET/SCI/RP/qIRS_NWC-157	1.0	31/01/22
[RD.3]	Algorithm Theoretical Basis Document for iSHAI Product Processors of the NWC/GEO	NWC/CDOP2/MTG/AEMET/SCI/ATBD/iSHAI	1.1	13/11/20
[RD.4]	Early adaptation of iSHAI v2016 to future MTG-I FCI using 2013 dataset	NWC/CDOP3/GEO/AEMET/SCI/RP01	1.0	31/01/20
[RD.5]	Validation Report for "Clear Air Products"	NWC/CDOP3/GEO/AEMET/SCI/VR/ClearAir	1.1	31/01/20
[RD.6]	Product User Manual for "Clear Air Products"	NWC/CDOP3/GEO/AEMET/SCI/UM/ClearAir	1.1	31/01/20
[RD.7]	Optimal use of MTG-IRS spectra on NWC SAF package for Nowcasting purposes	NWC/CDOP3/GEO/AEMET/SCI/RP/IRS_on_CDOP2	1.0	31/03/20
[RD.8]	Studies for comparison of NWCSAF/MSG PGE13 SPhR and IASI L2 products	NWC/CDOP2/GEO/AEMET/SCI/RP03	1.0	28/01/16
[RD.9]	Studies for the use of MTG-S/IRS L1 in nowcasting based in validation and training activities of the NWCSAF clear air products	NWC/CDOP2/GEO/AEMET/SCI/RP/02	1.0	30/11/14

Table 2: List of Referenced Documents

	Summary of activities of NWC SAF clear air team for preparation of MTG-S/IRS L2 from EUMETSAT in CDOP-3	Code: NWC/CDOP3/GEO/AEMET/SCI/JP/NWC-158 Issue: 1.1 Date: 11 March 2022 File: NWC-CDOP3-GEO-AEMET-SCI-RP-sSHAI_ES_NWC-158 Page: 14/46
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2 INTRODUCTION AND AIM OF THE STUDIES

The NWCSAF plan for supporting MTG-S/IRS is to offer a user friendly and optional software package to manage all MTG-S/IRS data and products for Day-2. This MTG-S/IRS IRS NWCSAF/GEO software package must be able to manage and to generate MTG-S/IRS L2 products files to get added value on all nowcasting products from the full MTG mission. One of the kind of MTG-S/IRS L2 products are the ones generated centrally on EUMETSAT headquarters by EUMETSAT Secretariat (ES) and disseminated by EUMETCast (satellite and terrestrial). Between these ES IRS L2 products are the retrieved temperature, humidity and ozone profiles, fields as skin temperature and emissivity atlases. These ES IRS L2 products are also of great interest for the use in nowcasting. By this reason it must be offered a NWCSAF service for the integration in the user local data cubes and to explore the possibility to use for generation of new products.

NWC SAF: CDOP-3 proposal


Version 1.0, 11 April 2016

WP ID 2630	Title of WP:	GEO-S v202X sSHAI_ES	
Start:	Mar-2017	Effort (mm):	5
End:	Feb-2022	Responsible partner:	AEMET
WP Objective/s	Development of management service from EUMETSAT Secretariat MTG-IRS L2 retrieved profiles disseminated by EUMETCast: calculation of Nowcasting parameters and reprojection to NWCSAF MTG-FCI regions.		
WP Tasks	<p><u>Development of the prototype tool for calculation of Nowcasting parameters from EUMETSAT Secretariat generated profiles disseminated by EUMETCast on user defined regions</u></p> <p>*) Construction of one prototype to read for every dwell inside user defined regions the T/q/O₃ profiles from EUMETSAT Secretariat MTG-IRS L2 files received by EUMETCast, calculate the Nowcasting parameters (with same algorithms that for MTG-FCI iSHAI parameters) and write the output with the same format as NWCSAF MTG-FCI iSHAI.</p> <p>*) Developments for optimal reprojection and dwells concatenation of Nowcasting parameters to user defined NWCSAF MTG-FCI regions and projection and writing on NWCSAF MTG-FCI iSHAI projection and format.</p> <p>*) Contributions for reviews.</p> <p><u>Comparison with iSHAI, validation activities and Users Training.</u></p> <p>*) Construction of one prototype to add EUMETSAT Secretariat IASI (or similar instruments) L2 products received from EUMETCast to the validation and training dataset of MTG-FCI and MTG-IRS L1 and L2 products.</p>		
WP Input	RTTOV software. McIDAS-V software (HYDRA) for IASI and MTG-IRS L2 management McIDAS-X software to test the reprojection software		
WP Output	EUMETSAT Secretariat MTG-IRS L2 products on MTG-FCI regions with Nowcasting parameters added (generated with the same algorithms used in NWCSAF/GEO SW Library). MTG-IRS scientific documentation (Scientific Report)		
WP Interfaces			
Interactions with other SAFS and/or Federated Activities	Coordination with EUMETSAT Secretariat on the format of MTG-IRS L2 files and other issues as navigation.		

4570

Figure 1: WP 2630 “GEO-S v202X sSHAI_ES” in CDOP-3 proposal [AD.1].

In CDOP-3 proposal [AD.1], it was planned to do the preparation of the products and services for a MTG-S/IRS IRS NWCSAF/GEO software package. In CDOP-3 proposal, the working package WP

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2630 “GEO-S v202X sSHAI_ES” was foreseen as activities to do at CDOP-3 phase (March 2017-February 2022); the wording of WP 2630 can be seen in Figure 1 (taken from [AD.1]).

The purpose of WP 2630 was to make preparatory developments of an operational service for management and support of EUMETSAT Secretariat MTG-S/IRS L2 products disseminated by EUMETCast and the integration in user local data cube on NWCSAF defined regions on MTG-I/FCI grid. This will allow to get a synergetic exploitation of the full MTG mission. From these developments a prototype would be obtained.

As commented above, a second guideline was to do all the activities in coordination and in synergetic way with the activities for preparation for MTG-I/FCI support. The MTG-S/IRS NWC SAF/GEO package must be designed and operated in a way that allows to explore the synergies and differences of MTG-S/IRS products, MTG-I/FCI products, MTG-I/LI and the NWP models.

As can be seen below, the management of the delivered ES IRS L2 puzzle on dwell by dwell files and some characteristics on the ES IRS L2 files implies the need of some software to make some basic operations. Between these basic operations are: the vertical interpolation from hybrid levels to a set of pressure levels, concatenation and reprojection from IRS dwell files, calculation (if needed) of same nowcasting parameters that in FCI L2 products and writing in files for user’s NWCSAF region of interest in adequate formats.

Thus, NWC SAF users with the instances of NWCSAF GEO software packages configured for MTG-I and MTG-S/IRS will be able to manage MTG-I L1 (FCI and LI) data, MTG-S/IRS L1 data, to generate MTG-I (FCI and LI) L2, MTG-S/IRS L2 products and to get their own collocated local data cubes on their region of interest.


The third guideline is the Coordination with EUMETSAT Secretariat on the content and format of MTG-S/IRS L2 files and other issues as navigation or slant representation.

For these reasons, it was designed WP 2630 with the main objective of the continuation of the development of the management service from EUMETSAT Secretariat MTG-S/IRS L2 products disseminated by EUMETCast.

As it is commented in Chapter 3 some circumstances have modified the activities made. It must be taken into account that due to the SAFs five year scheduling basis, at the moment when the proposal for CDOP-3 was written in 2016 the schedule of the launches of MTG-I/FCI and MTG-S/IRS was different. The launches on MTG mission have been delayed several years and MTG-I and MTG-S will be launched finally in CDOP-4.

In relation with the tasks proposed in the WP they have been slowed down mainly due to the lack of EUMETSAT Secretariat sample L2 files in the format disseminated by EUMETCast.

When the CDOP-3 proposal was written in WP 2630 it was foreseen the continuation of the “*development of the prototype tool for calculation of Nowcasting parameters from EUMETSAT Secretariat generated profiles disseminated by EUMETCast on user defined regions*”. This task was proposed thinking on a continuation of the EUMETSAT MTG-IRS NRT Demonstration Project; see Section 3.1.1 for more details. Due to the cancellation of the EUMETSAT MTG-IRS NRT Demonstration Project it was not possible to make the update of the clear air team software from the first phase of MTG-IRS NRT Demonstration prototype in order to advance on getting an operational prototype.

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The other possibility to follow with the improvement of the prototype was that EUMETSAT provided sample IRS L2 files. But in CDOP-3, EUMETSAT has not provided till now sample IRS L2 files; only it has been distributed through IRS MAG Group some documentation (ATBD and format content) with the foreseen content of IRS L2 files.

Due to these facts, the task to build an sSHAI_ES prototype has been slowed down. In the meantime, instead of developing the prototype it has been advanced in the developing of the functions and methods needed to build it. Between the advances in the development of the components made in CDOP-3 phase are the 4D interpolation and the reprojection. These activities are shown in Chapter 3.


In relation with the task to create a first collocated dataset with: IASI L1 spectra, IASI L2 retrieved profiles, SEVIRI or FCI NWCSAF products and ECMWF profiles from several forecast steps and nearest analysis this activity was linked to the second edition of the EUMETSAT MTG-IRS NRT Demonstration Project. But due to the cancellation of the second phase of the EUMETSAT MTG-IRS NRT Demonstration Project, this task was reduced initially to create datasets from IASI L1 and IASI L2 netCDF files from EUMETSAT UMARF for just several case studies. In the last part of CDOP-3 phase, this activity has been superseded also by the generation of synthetic IASI, IRS, FCI and MSG data together with the generation of the 4D data cube with the profiles used for the synthetic data generation; see documents [RD.1] and [RD.2]. More details are provided in Section 3.4. Through the use of the synthetic FCI, IRS and IASI datasets some of the uses of the proposed addition of IASI L2 and IASI L1 to the IRS, MSG and FCI validation and training dataset are not needed; because many of the tests foreseen could be done better with the use of the input profiles to RTTOV as a truth.

In Section 3.4 it will be shown how some of the developments in PGE00* tools would be used in CDOP-4 to generate to the future training validation datasets with collocated real and synthetic IRS, FCI and IASI data. Also PGE00* tools could adapted to add collocated synthetic IRS, FCI and IASI data and the profiles from 4D NWP interpolated to the pixels in the datasets; this activities could be started in MTG commissioning phases. Also the routines on PGE00* tools could be adapted to add EUMETSAT Secretariat IRS L2 products received from EUMETCast to the validation and training dataset of the future MTG-I/FCI and MTG-S/IRS L1 data and L2 products. This improved training and validation dataset will be used for tuning to the algorithms with real data, comparison of algorithm performances from real and synthetic data, generation of validation statistics and for bias BT corrections.

It is important to note that the use of synthetic FCI data as input to NWCSAF/GEO software and the generation of the synthetic NWCSAF products (see [RD.1]) has allowed to create software that could be used using the “back door” trick to made parallel tests to explore also the developments of software and products using blended FCI and IRS data and products. This will allow to make tests for the comparison of the use as input to FCI PGEs of IRS L2 fields instead of NWP fields. As example, it could be make the comparison of the use of IRS L2 SKT field instead of the use of a forecast NWP SKT field. Also it could be made tests for the use in iSHAI of sSHAI_ES IRS L2 emissivity atlases (instead of the static RTTOV emissivity atlases).

sSHAI_ES IRS L2 fields could be used by the users for near real time validation activities through the comparison of nowcasting parameters from iSHAI with equivalent parameters from NWP; some examples are shown in Chapter 3.

In relation with “Contributions for reviews” it has been contributed to the revision to the ATBD of EUMETSAT IRS L1 and L2 and the format documentation through the participation on the IRS MAG Group. The NWCSAF has also contributed to the MTG-I STRR Review and the use of PGE00 adapted to the STRR MTG NWCSAF library has allowed to generate the synthetic FCI and IRS dataset on the future MTG-I/FCI grid on geostationary projection; see [RD.1] and [RD.2].

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In CDOP-3 other documentation activities has been the presentations on the use of MTG-S/IRS L2 on nowcasting using the NWC SAF packages through:

- The participation on several workshops and Conferences. The presentations are listed in the Chapter 5 References and in the [iSHAI References](#) web page. The links to the presentations in pptx format are provided in both References lists.
- The participation on the IRS MAG (Mission Advisory Group). The presentations are also available in the EUMETSAT web.
- This Report is another opportunity to do it and to provide a summary of the activities.

It is expected that once MTG-II is launched and advanced the commissioning phase more effort and activities will be dedicated to prepare MTG-S1 launch by EUMETSAT. On this horizon, more and better test data will be delivered by EUMETSAT and one or more set of dwell files will be available; then, it will be resumed the preparation of reprojection and concatenation prototype.

As it will be shown through this Report, the activities for preparation for MTG-S/IRS are based and made in parallel with the ones for iSHAI (imager Satellite Humidity And Instability).

2.1 MTG-S/IRS ON NWC-SAF

The main objective of the NWC SAF is to provide software packages to ensure the optimal use of meteorological satellite data in Nowcasting and Very Short Range Forecasting. By this reason, the NWC SAF is one special SAF because it develops and provides software. Since NWCSAF products are generated locally by users this implies that there are no bandwidth constraints on local generated products. As can be seen in Figure 2, it works in the user's side of the EUMETCast. For this reasons, NWC SAF is the SAF nearest to users.

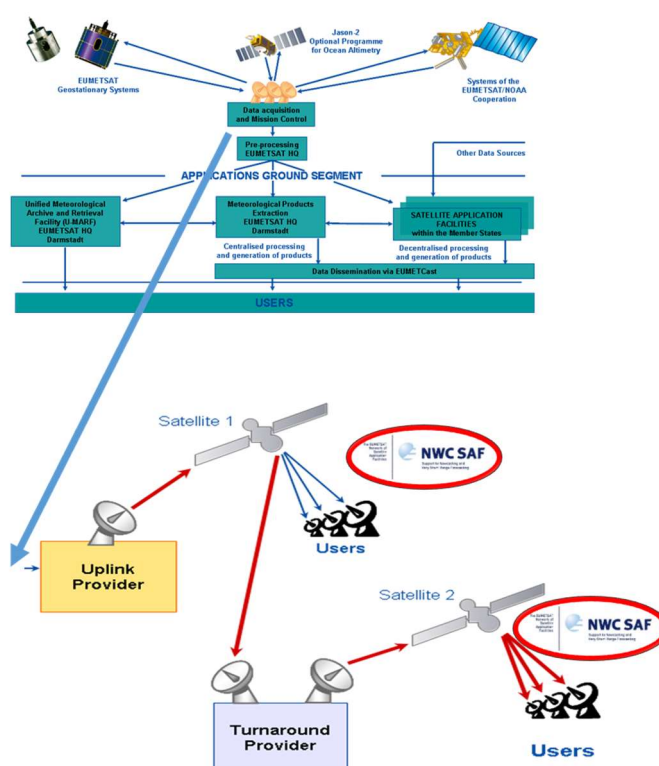



Figure 2: NWCSAF software is installed and executed on the user side of the EUMETCast.

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2.2 PROPOSED NWCSAF IRS PRODUCTS AND SERVICES

As can be seen if Figure 3, for MTG-S/IRS are foreseen three products and services:

Quick-IRS L1: support of the MTG-S/IRS L1 activities related to the local generation of simple image type products and to the generation of inputs for local generation of NWC SAF or users products.


Since EUMETSAT will disseminate by EUMETCast satellite just 300 Principal Components in 160x160 pixels dwell files, this service/product will made the following steps:

- A) IRS BTs spectra reconstruction from the 300 Principal Components for every pixel on every needed dwell file to cover the user region of interest.
- B) For every MTG-S/IRS L1 channels in one users configurable predefined list, it will made the combination and reprojection from the needed dwells files to user NWC SAF regions on a geostationary grid (by default the IR FCI grid on 2x2 boxes). This is needed because the disseminated EUMETSAT dwell files are not reprojected to a fixed grid and just latitude and longitude matrices are included in the dwell files.
- C) Finally some easy IRS image type products will be generated. As an example, the following could be generated:
 - MTG-S/IRS RGB images
 - Normalized IRS-L1 channels in some spectral regions (as CO₂ or WV branches) representing the state of the atmosphere at several layers.
 - Simple operations with MTG-S/IRS L1 as difference or regressions between several IRS L1 channels. It could be also tested the outputs of simple Machine Learning algorithms.

Thus, users could made the automatic generation of IRS L1 imagery related products or to use them for locally generation of NWC SAF or users products. See also Chapter 5 References for some examples.

sSHAI ES: support of the MTG-S/IRS L2 files disseminated by EUMETSAT Secretariat (ES) by EUMETCast. sSHAI_ES software is needed because EUMETSAT will disseminate the centrally generated ES IRS L2 files by EUMETCast on dwell by dwell files and they are not reprojected to a fixed grid (just latitude and longitude matrices are included in the dwell files). Thus, 2D and 3D fields read from the IRS L2 dwells files will be combined and reprojected to users NWC SAF regions. Every dwell file will have 160x160 pixels. The spatial resolution on IRS L1 and L2 files is roughly equivalent to 4x4 km on nadir; this spatial resolution is roughly equivalent to a box of 2x2 pixels on MTG-I/FCI grid. Since the subsatellite points of MTG-S (3.4° E) and MTG-I (0°) are very close, a natural choice is to try to reproject the IRS L2 fields to FCI grid; it could be configurable the choice to do in boxes of 1x1 or 2x2 of FCI IR pixels. Taking these into account these service will made the following main steps:

- Vertical interpolation from hybrid levels to a configurable set of fixed pressure levels.
- Calculation of several nowcasting parameters (TPW, LPW and instability indices) will be made also if there are not included in the EUMESAT L2 files.
- The combination and reprojection from needed dwell files to user NWC SAF regions on a geostationary grid; by default 2x2 boxes of IR FCI grid.

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- Thus, 2D and 3D fields read from the IRS L2 dwells files will be combined and reprojected to users NWC SAF regions.
- Writing on netCDF format with a design as much compatible as possible with standard meteorological tools.

The idea is that ES MTG-S/IRS L2 fields could be used then directly by users in combination with the ones from MTG-I/FCI fields for same regions. As an example, the comparison of instability indices from MTG-I/FCI, MTG-S/IRS and NWP.

Also, the sSHAI_ES IRS L2 fields on NWCSAF region could also be used in a future as input to locally generated products. As an example, IRS SKT field or IRS emissivities could be used as input for MTG-I/FCI product in future versions. See more details on [RD.2].

sSHAI: development of product executed locally by the users. Local generation of NWCSAF MTG-S/IRS L2 product using light demand CPU algorithms.

- The first product of this type is the local retrieval of T, q profiles using as additional input local NWP models (executed using light CPU algorithms) for a set of selected dwells. At this moment, the NWC SAF team is developing an algorithm that use kernel ridge regression trained with IASI L1 and NWP analysis of the previous day using a rolling training approach.
- Calculation of nowcasting parameters (TPW, LPW and Instability indices) at dwells.
- Then, combination and reprojection from dwells to user NWC SAF defined regions.

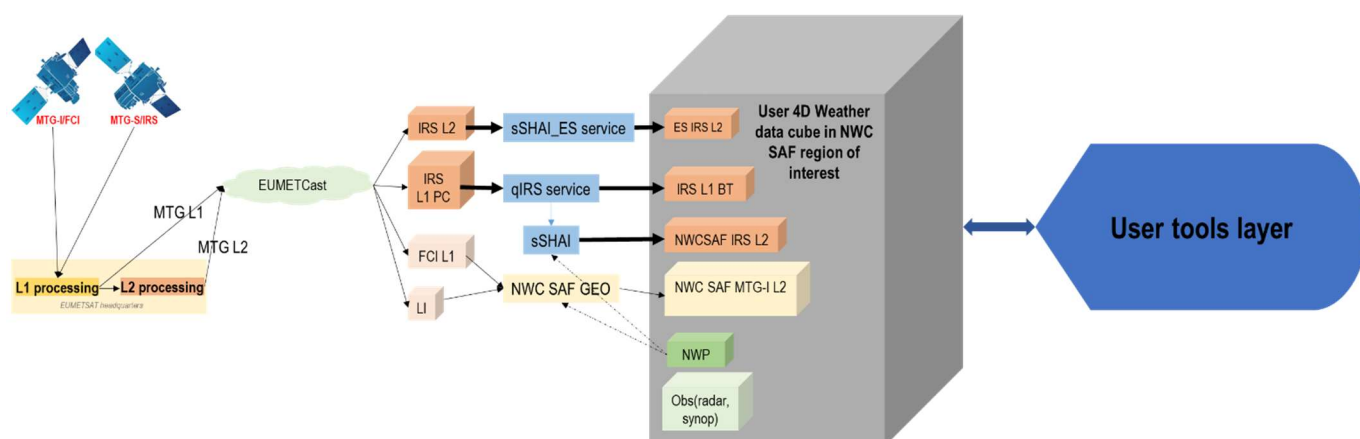



Figure 3: Scheme of the proposed NWCSAF/GEO services and products for MTG-S/IRS. The users will have the possibility to create their own 4D weather data cube in their region of interest. As proxy of user tools layer able to manage all the types of the L1 and L2 files it has been used McIDAS-V in this Report.

The MTG-S/IRS NWC SAF/GEO package will be prepared during CDOP-4 and they will be available at Day-2.

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3 CHAPTER SSHAI_ES: SOUNDER SHAI FROM EUMETSAT SECRETARIAT (ES) MTG-S/IRS L2 SERVICE:

Some activities made in CDOP-3 related with the use of other L2 netCDF files from hyperspectral instruments as proxy of future IRS L2 are commented in this Chapter. The issues raised and the proposed solutions will contribute to the final objective to get a design of the adaptation of EUMETSAT L2 files in sSHAI_ES L2 files with a more adequate netCDF format for users and for nowcasting purposes. It is also described the way that it has been developed and improved all the components for the tools that will be used in CDOP-4 for the development of the software for sSHAI_ES service using other sources of L2 files.

As commented previously, at the time to write this Scientific Report MTG example or test IRS L2 files has not been distributed by EUMETSAT.

In Section 3.1 it is summarized the activities related to the use of IASI L2 products files for preparation of IRS L2. In Subsection 3.1.1 are described the activities related to the participation in the EUMETSAT MTG-IRS Near Real Time (NRT) Demonstration Project; it is shown how some of the tools developed on the participation in the NRT IRS Project are the basis for some of the components for the future preparation of the sSHAI_ES prototype. It has been also used UMARF IASI L2 files as proxy of future MTG-S/IRS L2 files; see Section 3.1.2. This activity has involved the update of the old IDL converter programs and they will be used as basis for more developments in CDOP-4 phase to be ready for MTG-S launch. The expertise on the use of real IASI L1 and IASI L2 netCDF files from EUMETSAT at the beginning of CDOP-3 has been shown on Martinez presentations (2018b, 2018a, 2020a) and a broad summaries are available also in [RD.7], [RD.8] and [RD.9]. Then after check that they cannot be used direct and interactively by the users it was written some IDL/GDL converter programs in order to write the IASI netCDF files compatible with McIDAS-V.


In CDOP-3 it was foreseen to make advances in the reprojection to NWCSAF MTG-I/FCI regions. The activities related to the optimal reprojection procedure and dwells concatenation of nowcasting parameters to user defined NWCSAF regions are shown in Section 3.2. It is shown the proposed remapping algorithm. Together with the use of this remapping algorithm with IASI L2 files it has been used also files from Sentinel mission. The use of remapping together with the programs to write on McIDAS-V compatible netCDF files has allowed the intercomparison of products from MSG iSHAI, ECMWF, IASI L2 and Sentinel mission; see the examples in Section 3.2.

In Section 3.3, it is made a summary of the proposed sSHAI_ES service.

In Section 3.4, are described the PGE00* tools and how they have been used to create synthetic datacubes. It will be used as basis for the generation of MTG-I/FCI and MTG-S/IRS collocated datasets with real data together with the synthetic datasets twins from the NWP nearest analysis. Other value add of these synthetic FCI and IRS datasets is that have been generated on collocated time and regions allowing to explore a full synergetic exploitation of FCI and IRS data.

3.1 ACTIVITIES RELATED TO USE IASI L2 AS PROXY OF MTG-S/IRS LEVEL 2 USE

In this Section are described some previous activities with IASI L2 files as proxy of future ES MTG-S/IRS L2 files. The most important are related to experiences and lesson learned from the participation on the MTG-IRS Near Real Time Demonstration Project and the use of IASI L2 files downloaded from UMARF for several case studies.

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3.1.1 Participation on the EUMETSAT MTG-IRS NRT Demonstration Project

The clear air NWCSAF AEMET team participation on the EUMETSAT MTG-IRS Near Real Time (NRT) Demonstration Project was initiated at end 2015 after an invitation of at that time responsible of MTG-S/IRS, Stephen Tjemkes, and the responsible of the MTG program Rolf Stuhlmann.

In the EUMETSAT MTG-IRS NRT Demonstration Project, IASI data from METOP-A and B over Europe were processed in NRT mode with the at that time prototype for EUMETSAT MTG-IRS L2 algorithm. At that time, the algorithm was based in physical retrieval using as First-Guess (FG) the ECWMF model. Thus, EUMETSAT MTG-IRS NRT Demonstration Project products could be considered as a source of proxy MTG-S/IRS data to build a training dataset in accordance with proposed AEMET NWC SAF CDOP-2 activities for MTG-S/IRS preparation.


The NWCSAF AEMET contribution in the project was based in the developing and operation of a chain triggered by a *crontab* that made the download from EUMETSAT ftp server, the read of IASI (MTG-S/IRS proxy data) files inside of the AEMET region of interest around Iberian Peninsula, the combination of several files in the region and the writing in a netCDF format compatible with the McIDAS-V tool. Thus, the MTG-S/IRS proxy products could be used and compared with other L1 and L2 products (NWP, NWCSAF iSHAI products from MSG, sSHAI from IASI prototype and UMARF EUMETSAT-ES IASI L2 v6.2 products). The process at AEMET was similar to the proposed sSHAI_ES service for the future disseminated EUMETSAT Secretariat MTG-S/IRS L2 products and the integration on the NWCSAF GEO software package.

In CDOP-2 phase, during the first phase of EUMETSAT MTG-IRS NRT Demonstration Project it was created a first version of programs to read every IASI L2 file from the experiment, convert the profiles from hybrid levels to a set of pressure levels, calculate the Nowcasting parameters (with same algorithms that for iSHAI parameters) and write the output with similar format that NWCSAF iSHAI format. More details are provided in [RD.7].

In 2017 it was started an offline reprocessing of all files in MTG-S/IRS NRT demo project to solve the issues of the aged ECMWF profiles as FG in NRT processing. In the reprocessing phase the ECMWF supply to the chain run successfully and IASI reprocessed L2 products was better. Some of the results were presented at the MTG-IRS NRT Demo Project Review Meeting the 18th-19th May 2017 in EUMETSAT; more details are provided in [RD.7].

When the tasks of WP 2630 for CDOP-3 proposal was written, it was foreseen the continuation of the EUMETSAT MTG-IRS NRT Demonstration Project. It was foreseen a second edition of the EUMETSAT MTG-IRS NRT Demonstration Project. But due to the retirement of Rolf Stuhlmann (the MTG program responsible at that time), the second edition was cancelled on January 2018. Also it was changed the IRS L2 algorithm from the use as FG of the ECMWF model to the use of PWLR³ regressions (as in the case of IASI L2 algorithm). Since the EUMETSAT MTG-IRS NRT Demonstration Project was stopped, the proposed modifications to the EUMETSAT processor (e.g. better description of the First Guess, improvement of the physical retrieval algorithm, improved netCDF design, etc.) was not implemented. By these reasons the update of the software of the clear air team for the first phase of MTG-IRS NRT Demonstration prototype was stopped.

In Figure 4 it can be seen an example of what could be get by users when sSHAI_ES fields will be used in future for comparison of the same nowcasting parameter from several sources; it has been used as example the precipitable water in the medium layer (850 to 500 hPa). Top of the Figure 4 are the ML fields calculated from IASI (from EUMETSAT MTG-IRS NRT Demonstration Project) FG and physical retrieval. As in the EUMETSAT MTG-IRS NRT Demonstration Project was retrieved only on clear air it has been used the McIDAS-V to overlap in grey levels an image of MSG IR10.8 (10:30Z)

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on the cloudy pixels detected NWCSAF MSG/SEVIRI Cloud Mask (CMA); this IR108 image is included in the MSG iSHAI files. These IASI ML fields can be compared with the same calculated from the ECMWF and MSG/SEVIRI iSHAI (bottom images). As all the parameters are in the same projection, with the same colour palette and the grey image cover the holes due to no processed pixels and provides the clouds pattern structure the Figure provides a good way to search for agreement and disagreement between the forecast and the real data and for the detections of the differences between IASI and MSG algorithms performances.

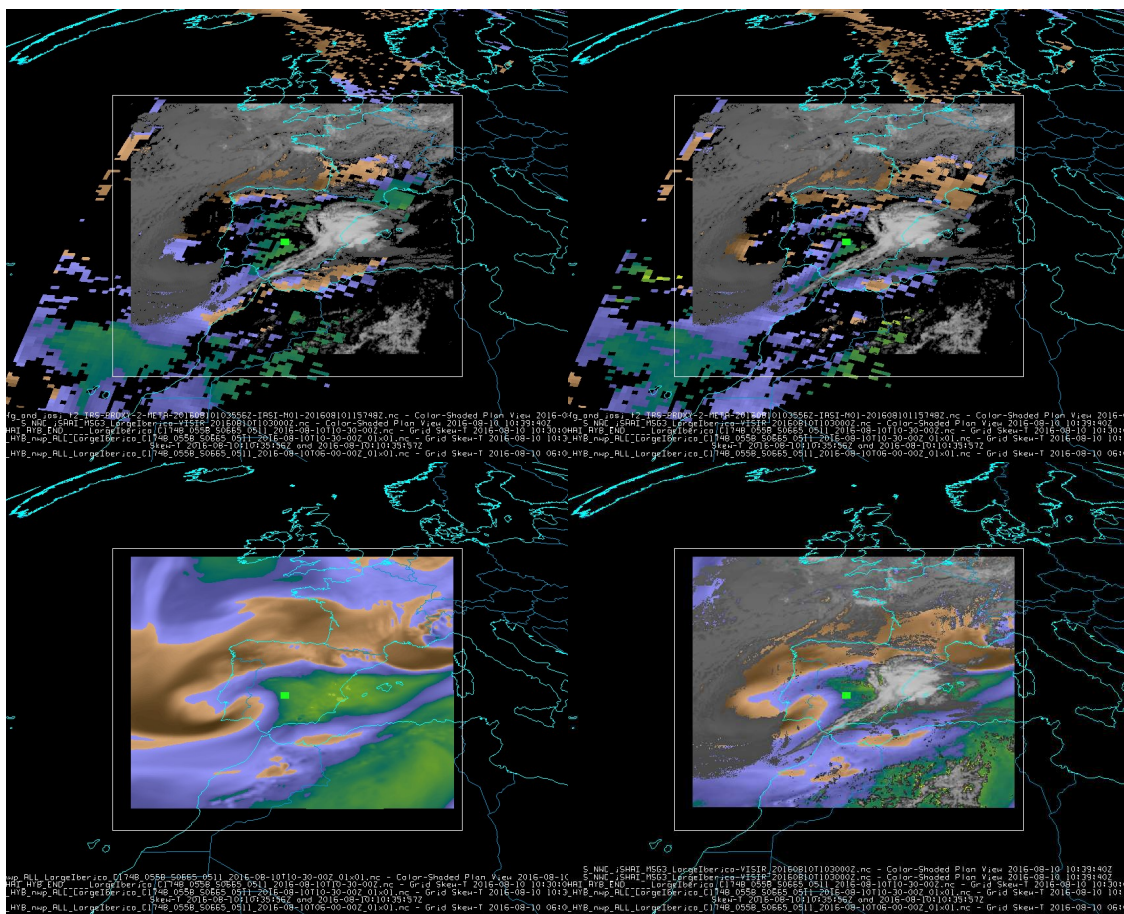


Figure 4: Precipitable water in Medium Layer (850 to 500 hPa) ML parameter calculated (top left) from FG IRS_proxy (top right) from physical retrieval FG IRS_proxy (bottom left) from ECMWF t+10:30Z forecast 4D interpolated using PGE00 tool (bottom right) from MSG iSHAI. Date: 10th August 2016 at 10:30Z; IASI orbit are 10:35Z. Overlapped in grey MSG IR10.8 (10:30Z) on cloudy pixels detected NWCSAF MSG/SEVIRI Cloud Mask (CMA). It has been used same colour palette.

3.1.2 ACTIVITIES WITH THE OFFICIAL EUMETSAT IASI L2 NETCDF FILES FROM UMARF.

As can be seen in References and in Martinez 2016c presentation, it has been downloaded in CDOP-2 from UMARF some EUMETSAT IASI L2 files for several cases studies to investigate their use in nowcasting. It is possible to download from EUMETSAT UMARF archive the IASI L2 files in native or netCDF-4 format. One of the key aspects for the use in nowcasting is the need of hyperspectral L2 files should be compatible with adequate exploitation and visualization tools. But in any of the cases

the UMARF IASI L2 files cannot be used as input to standard display and management tools due to lack of adequate design. As proxy of future user tools it has been used here the McIDAS-V tool.

The problem of UMARF IASI L2 netCDF-4 files is that they have been designed just as transcript from binary to netCDF format without taking into account any rule or convention in order to be compatible with any standard visualization tool. As in case of UMARF IASI L1 (see [RD.7]), this imply that they only can be read using ad hoc programs or program environments as Python, IDL, MATLAB, etc. Since these EUMETSAT UMARF IASI L2 files cannot be used by any standard application, the first activity was to develop a converter program to read the content from the EUMETSAT UMARF IASI L2 netCDF file and to convert it to a netCDF file with one internal design that could be used as input to McIDAS-V tool.

In the first attempts (in CDOP-2 phase) there was a bug in the UMARF transcript of IASI L2 from native to netCDF format. After EUMETSAT fixed the bug in the UMARF software, in November 2018 it was downloaded other time from UMARF the IASI L2 files for the same case study. In the Figure 5 it is shown the ML fields (precipitable water in Medium Layer) after conversion to McIDAS-V compatible netCDF files; the case study is the same that in Figure 4. In this case the FG field is available in all the pixels because is used the $PWLR^3$ algorithm; this is similar to the proposed now for IRS L2.

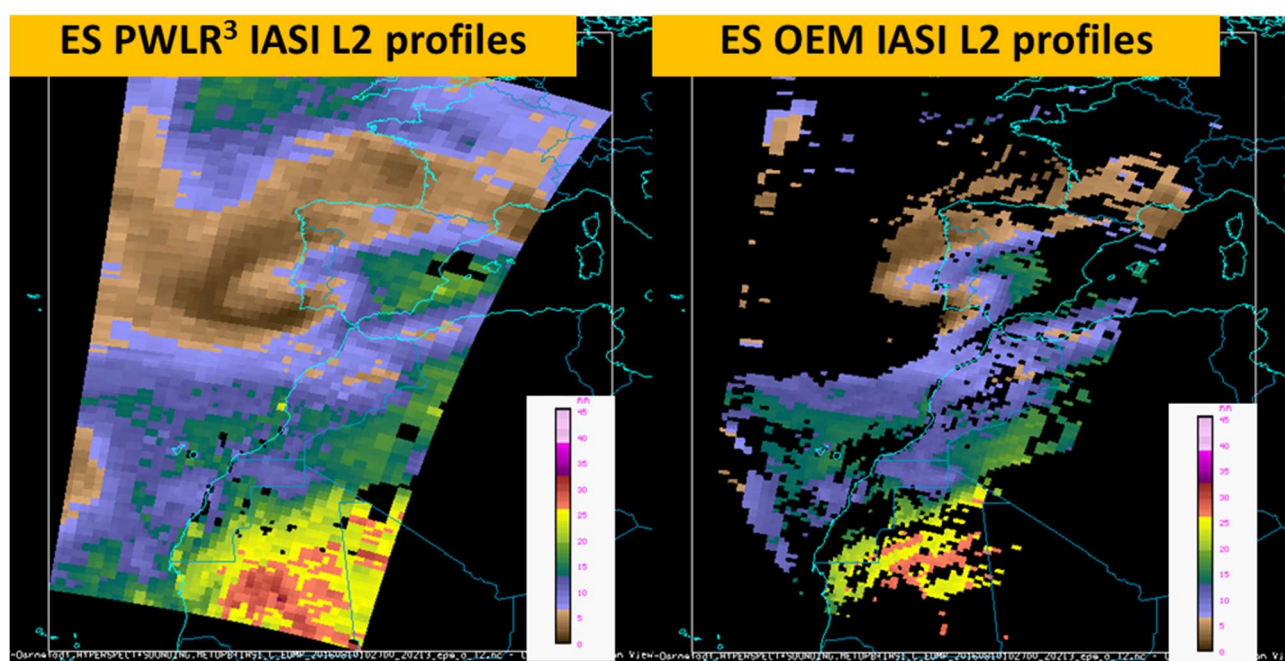



Figure 5: ML from METOP-B IASI L2 v6.2 profiles. (left) IASI L2 v6.2 $PWLR^3$ FG and (right) IASI L2 v6.2 optimal estimation. Images generated with McIDAS-V. 10th August 2016 \approx 10:33Z.

Also, due to that at AEMET the IDL version was very old (IDL version 6.2) the netCDF-4 files could not been read with it. As in the case of the prototype to read the EUMETSAT MTG-IRS NRT Demonstration Project files, it was updated the previous version to start to use the GDL HDF-5 functions to read the content of the netCDF-4 files and write it on binary files; these binary can be easily read on IDL (or GDL) using the command *restore*. Since GDL it is a GNU free clone of IDL, it was installed at AEMET and programs on GDL was started to be used as one step in the converter *script*; but the rest of the steps continued to be done with UNIX and IDL programs (due to some

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limitations on GDL). In autumn 2018, the GDL/IDL converter script was improved and updated with the lessons learned in the EUMETSAT MTG-IRS NRT Demonstration Project. It was added the following improvements:

- ✓ The interpolation from the 137 hybrid levels on IASI L2 files to a customizable array of fixed pressure levels in the converter. Together with the better use by user of arrays in pressure levels this fact allows also to reduce the size of the arrays in the compatible McIDAS-V netCDF file. The reduction on the size improves later the behavior on interactive displays because it is reduced the need of memory; especially if there are eliminated very high levels (as example, the profiles could be limited to levels with pressure greater than 200 hPa).
- ✓ The reorder IASI L2 pixels depending on the IASI detectors order (see [RD.7]). The EUMETSAT IASI L1 and L2 files are written not thinking in to be exploited as image arrays. If the use is for NWP or for just plot the data order is not important, but if the use is for display as image field it is crucial to reorder the data to be aligned as continuous arrays (see [RD.7]). That it is other example of the need of software in the users' side of EUMETCAST to cover the gap between EUMETSAT disseminated files and users' needs.
- ✓ Also the same parameters that in NWC SAF iSHAI product are calculated.

Early results was first shown on November 2018 IRS MAG meeting in Brussels; see Martinez 2018b.

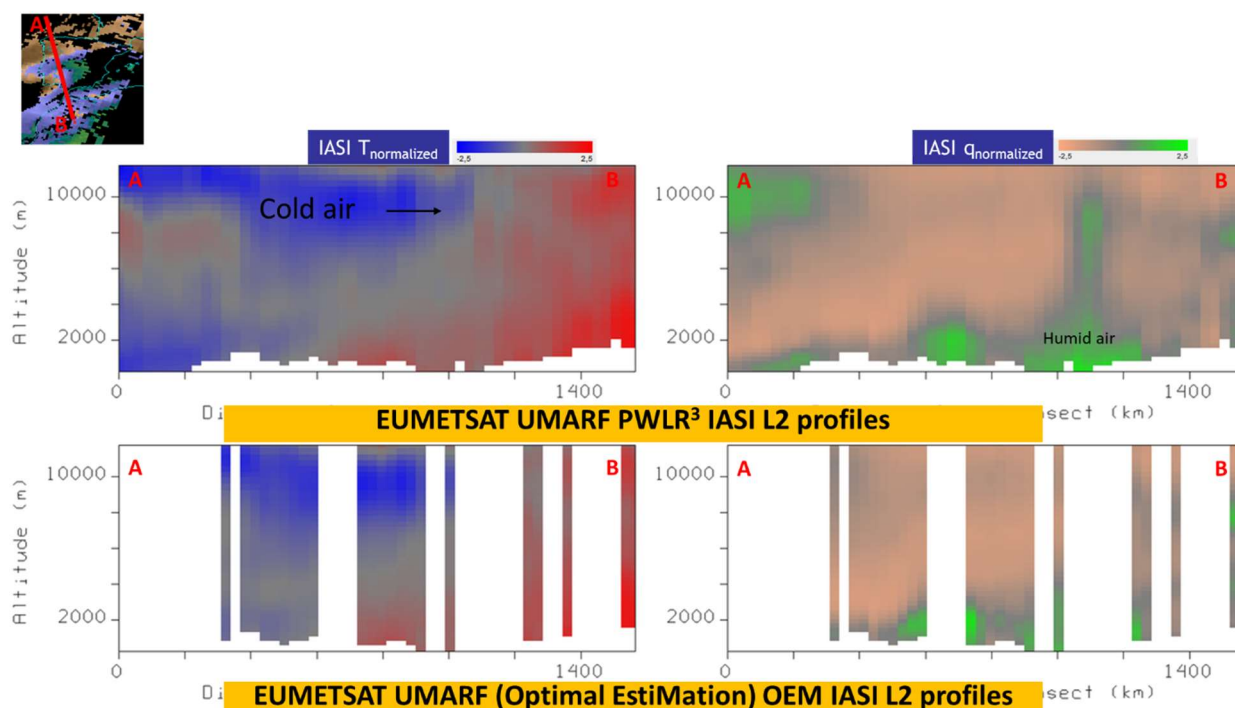


Figure 6: Example of vertical cross sections from A to B points of normalized T and q from EUMETSAT UMARF IASI L2 profiles. (top left) PWLR³ IASI $T_{normalized}$ (bottom left) Optimal Estimation (OEM) IASI $T_{normalized}$. (top right) PWLR³ IASI $q_{normalized}$ (bottom right) Optimal Estimation (OEM) IASI $q_{normalized}$ 10th August 2016 \approx 10:33Z. Blue (red) colors indicates colder (warmer) than the mean in the layer. Green colors indicates wetter than the mean in the layer.

Other brain storm idea (see Martinez [2013, 2015 and 2016]) is to add in future meteorological tools some interactive graphical support to represent at the same time profiles and normalized profiles or collocated NWP representations. This kind of application can be easily configured in the proposed

sSHAI_ES service. In the 2018 converter it was also added the configurable writing of normalized T and q profiles in the compatible McIDAS-V netcdf. It can be seen in Figure 6 examples of normalized vertical cross sections similar to the shown in Martinez 2018b from ECMWF or iSHAI profiles; copy of the Martinez 2018b presentation is available in the EUMETSAT web and the link to the presentation in pptx format is available in Chapter 5 References. It can be seen the presence of colder air intrusion in upper levels travelling from A to B; when it reach the vertical of green spot with humid air in low levels (Guadiana and Guadalquivir valleys) is triggered the convection; see the loops of SEVIRI RGB images, iSHAI and ECMWF fields in Martinez 2018b presentation.

3.2 REMAPPING ALGORITHM

As can be seen in Figure 7 it will be needed several IRS dwell files to get an IRS field for a usual region of interest of one user. Due to the fact that the fields on every dwell file are provide on a non-fixed IRS grid (with just longitude and latitude arrays provided on every dwell file) and with changes in the positions between consecutives slots, one of the key components of the sSHAI_ES services will be the remapping from the non-fixed IRS grid to a fixed geostationary grid that by default could be boxes of 2x2 on geostationary MTG-I/FCI grid. Later, the remapped dwell files could be combined to create a combined and remapped field on user defined NWCSAF regions.

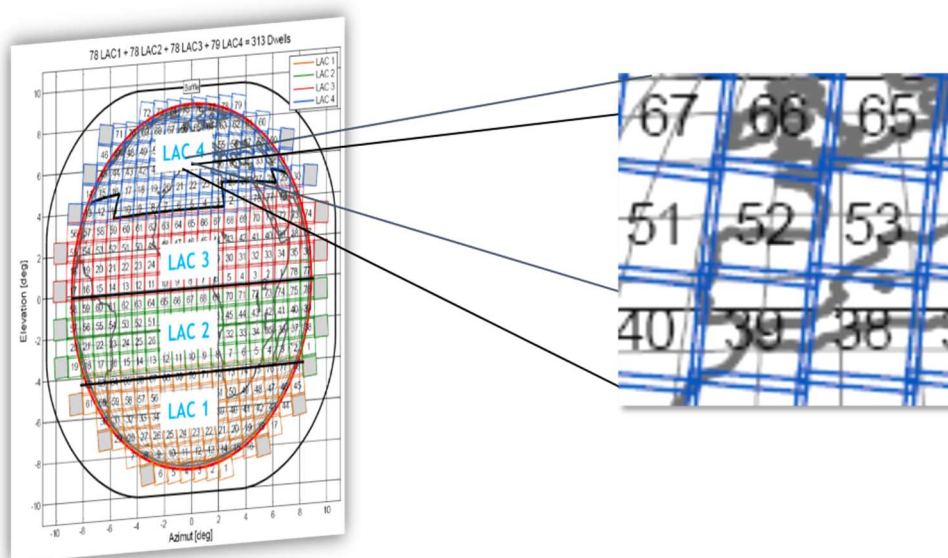



Figure 7: need of reprojection and combination of several dwells to cover a user' region of interest.

At the beginning of EUMETSAT MTG-IRS NRT Demonstration Project the first attempts for remapping required the calculation of the distance from every pixel in the target region (NWCSAF region on MSG grid) to all IASI pixels in every IASI file. This was due to lack of an inverse function to search the (line, column) in IASI matrix for given (latitude, longitude).

In the classic remapping algorithms (as for example in McIDAS-X since 90s) there are provided for every projection two functions:

- ✓ ll2xy: this functions makes the calculation of the (line, column) of a pixel in the projection defined grid using as input the (latitude, longitude) of the pixel.

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- ✓ xy2ll: this functions made the inverse. It makes the calculation of the (latitude, longitude) of a pixel in the projection defined grid using as input the (line, column) of the pixel.

In case not to have a direct formula or algorithm for the calculation the alternative is implement search strategies in arrays with the (latitude, longitude).

Once the two direct and inverse function are available the usual way in remapping is to make a nested loop and for each pixel in the destination grid:

- It is used the (line, column) as input to ll2xy function in target projection to know the (latitude, longitude) coordinates.
- It is used the (latitude, longitude) as input to xy2ll routine in the source projection to know (line, column) in source grid of pixel to be used as basis to perform the interpolation from source pixel to target pixel. It could be implemented nearest neighbor or bilinear or etc.

Using this base remapping algorithm there are a lot of hybrid approach to speed-up more the remapping; as example to make first for reduced set of pixels and use some interpolation, etc.

In the case of IASI (used as proxy of IRS on MTG-IRS NRT Demonstration Project) to MSG remapping the number of pixels is much higher in the target MSG grid this slows down the remapping. As in addition, in the EUMETSAT experiment it was only processed in clear air, the process was done for many unnecessary points. These facts could be used to considerably speed-up the remapping. Then, it was started the study of optimal and fast reprojection algorithm from IASI pixels (as proxy of MTG-S/IRS) to NWC SAF regions (subsets of GEO reprojection grid).

Using the reverse process of starting at IASI grid only for valid pixels could be diminish the number of operations by a large factor. For every processed IASI pixel, the (line, column) of IASI pixel provided the (latitude, longitude) of the pixel by reading them from longitude and latitude arrays read from the IASI L2 file. Then, the MSG xy2ll function quickly provides (line, column) in the MSG grid and it can be determined whether or not it is inside the NWCSAF region. The first version was developed and programed in 2017 spring and the scheme can be seen in Figure 8. The early prototype is written in IDL. It is based in:

- a) Search valid pixels in IASI array.
- b) For every valid IASI pixel uses the (longitude, latitude) of the 4 nearest IASI pixels and a function xy2ll(latitude, longitude) to get the corresponding (line, column) in MSG grid.
- c) The dimensions and position on MSG grid of the NWC SAF are used to calculate the (line, column) in the NWC SAF region for the 4 IASI corners.
- d) If the (line, column) with the corners positions are inside the NWCSAF region. For every GEO pixel between the corners the interpolation is performed using the coordinates of the nearby IASI pixels:
 - ✓ It is calculated the distances of the GEO pixel to the 4 IASI neighbors
 - ✓ It is calculated de value on GEO pixel as combination of the value in the 4 IASI neighbors weighted for the inverse of the square of the distances.

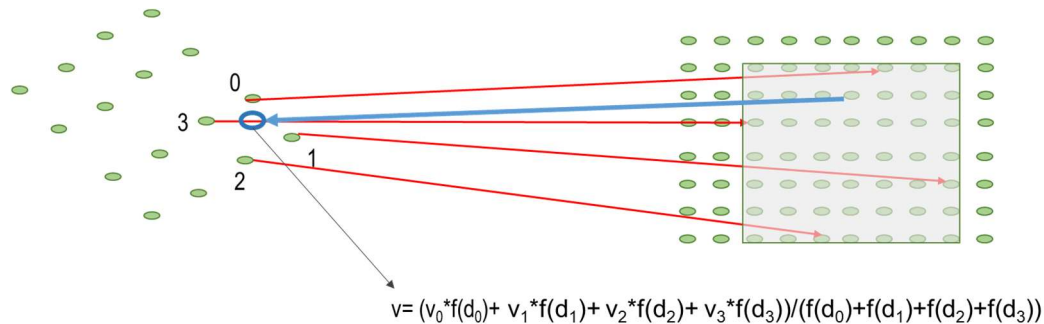


Figure 8: Scheme of fast interpolation proposed for remapping from IASI to MSG grid.

The first results using the proposed reprojection algorithm was shown in the last Workshop of EUMETSAT MTG-IRS NRT Demonstration Project in May 2017 (there are not public presentations). In the Figure 9 it can be seen one example of the remapped ML fields from the reprocessing of EUMETSAT MTG-IRS NRT Demonstration Project IASI L2 file for case study of Malaga flash flood in the early morning of 19 February 2017; they are compared with ECMWF and MSG iSHAI equivalent fields. This case study was used also in May 2017 in an internal AEMET meeting.

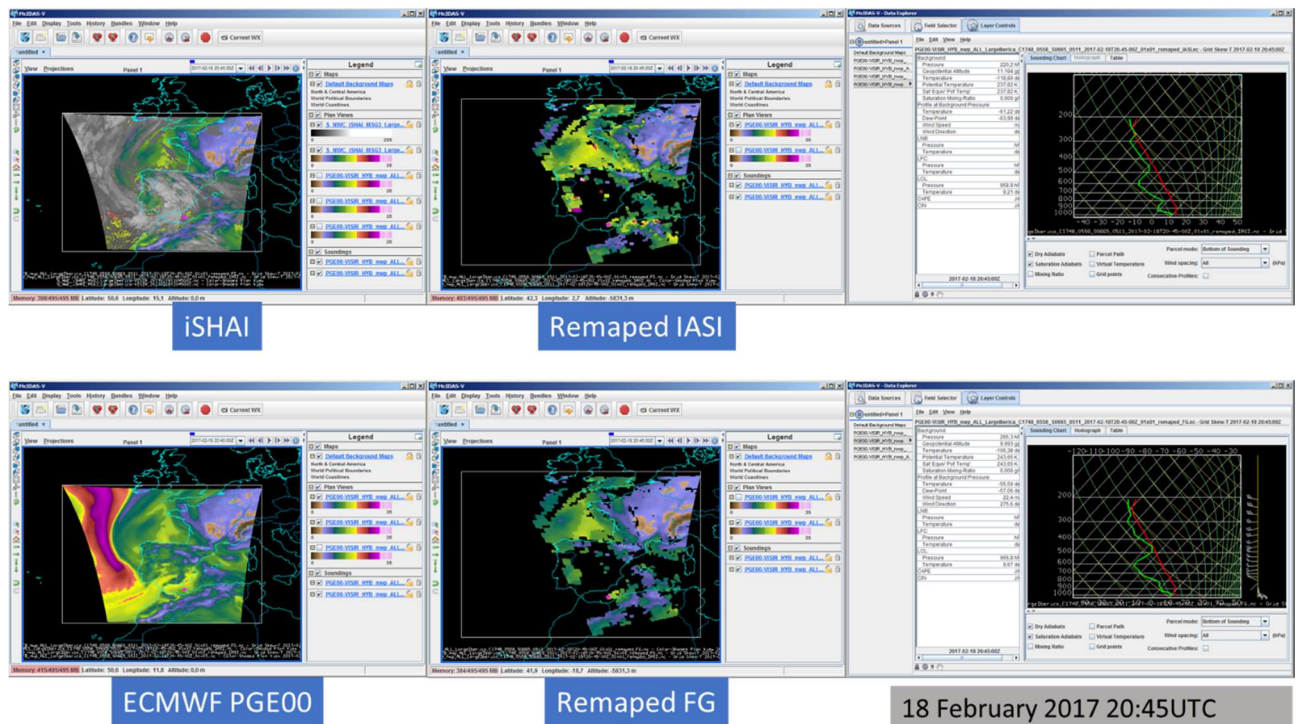



Figure 9: ML fields from EUMETSAT MTG-IRS NRT Demonstration Project IASI L2 file on reprocessing phase and the comparison with ECMWF and MSG iSHAI fields. Case study Malaga flood 19 February 2017.

Not only one 2D field it is remapped every time. Once it has been determined the pointers between the source and target grids and it has been calculated the weighting factors they are used also to make the remapping of the whole set of 2D and 3D fields. If the remapped fields are writing in compatible

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McIDAS-V netCDF files, they could be exploited for generation of display of sounding or 2D or 3D displays.

This early version of the IDL remapping prototype was optimized. The results of the use of the optimized remapping algorithm using EUMETSAT UMARF IASI L2 files were first shown on November 2018 IRS MAG meeting in Brussels. It can be seen in Martinez 2018b presentation; copy of the presentation is available in the EUMETSAT web and the link to the presentation in pptx format is available in References Chapter.

It was used the same EUMETSAT UMARF IASI L2 files used to generate the Figures 5 and 6 from case study 10th August 2016. This case study it is the same used as a reference several times for iSHAI and PGE00 in several presentations; see Martinez 2016 and 2018a. Due to this fact, in Figures 10 and 11 it can be seen another example of what could be get by users when sSHAI_ES fields will be used in future for comparison of the same nowcasting parameter from several sources.

In Figure 10 are shown the ML fields calculated from EUMETSAT UMARF IASI L2 product (PWLR3 First-Guess in all pixels and Optimal Estimation on clear air pixels) after reprojection to the same NWCSAF region and projection on MSG/SEVIRI grid that SEVIRI iSHAI and ECMWF (PGE00) ML fields. It can be seen one agreement in the spatial pattern and structures.

Since the ML fields have same dimensions and projection it could be used on McIDAS-V to calculate on the fly the differences versus from $t+10:30$ forecast ECMWF ML field. After display those in same colour palette the difference ML fields could be used to estimate the change in the background NWP introduced by SEVIRI iSHAI and compare with the NWP free estimation from IASI L2 algorithms. The IASI difference ML fields agrees with MSG/SEVIRI iSHAI ML on the overestimation on ML in the ECMWF in the region of interest of Betica region where severe storms were triggered when cold air in upper levels reach the Betica region with moist air in low levels.

Using on McIDAS-V the remapped IASI L2 netCDF file it is possible to do interactive exploitation with 2D or 3D displays (vertical cross section, etc.). Also the differences versus NWP and MSG could be made on the 3D and 4D datacubes to explore the vertical difference structures. As an example a video with the screen capture of an interactive McIDAS-V comparison of vertical cross section with the difference in q 3D arrays from ECMWF and IASI L2v6 can be seen in Martinez 2018b slide 39.

Till now it has been used NWCSAF MSG/SEVIRI grid but in CDOP-4 it will be updated to MTG-I/FCI grid. Some of the functions from the remapping algorithm have been used as basis generation of synthetic datasets using as input combined Harmonie NWP model and ECMWF operational GRIB on hybrid files; see [RD.1] and [RD.2].

In 2020, as it can be seen in next subsections this remapping algorithm has been used several times with Sentinel satellites files.

By the moment it is not possible to advance more in the algorithm because through the participation in the IRS MAG it is know the existence of some open issues that should be taking into account:

- ✓ EUMETSAT Secretariat wants to make the IRS L2 retrieval using slant views.
- ✓ To avoid solar intrusions in the IRS instrument the satellite is yaw flipped two times per year; this will make the arrays could be rotated 180° during a half of the year.
- ✓ Also this remapping algorithm will be used for remapping IRS L1 fields and the LWIR and MWIR bands which are slightly shifted.
- ✓ If there were an inverse function, it would not be necessary some this remapping algorithm.

As summary more activities will be made when EUMETSAT deliver IRS L1 and IRS L2 sample files.

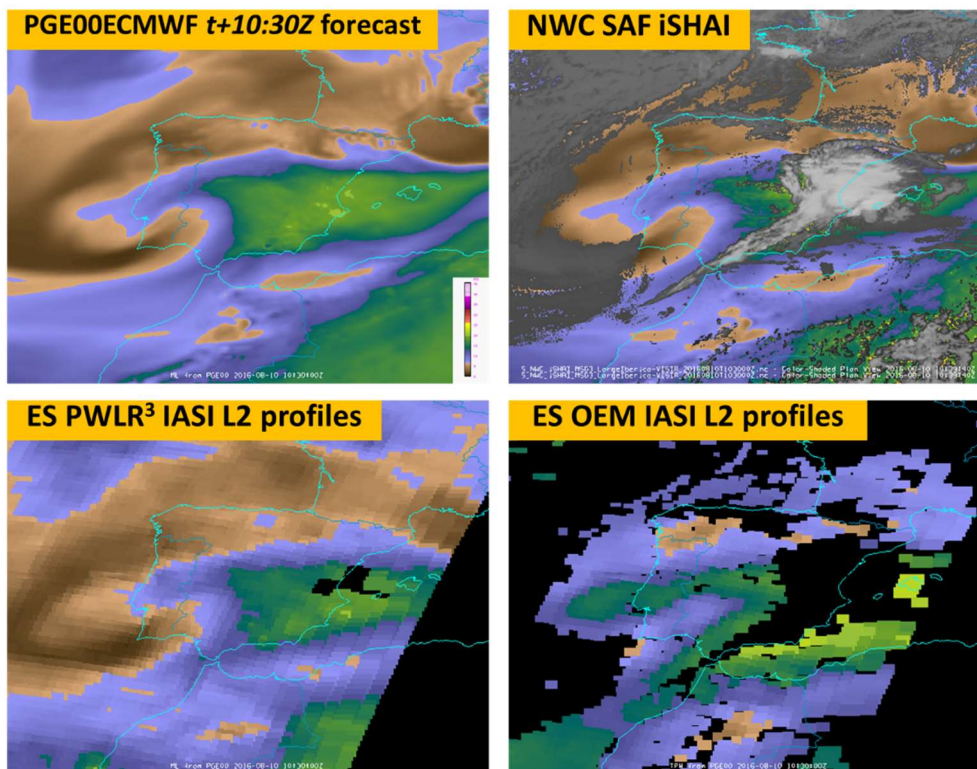


Figure 10: ML from (top left) ECMWF t+10:30Z forecast (top right) MSG iSHAI 10:30Z. (bottom left) ES PWLR³ IASI L2 (bottom right) ES OEM IASI L2. 10th August 2016.

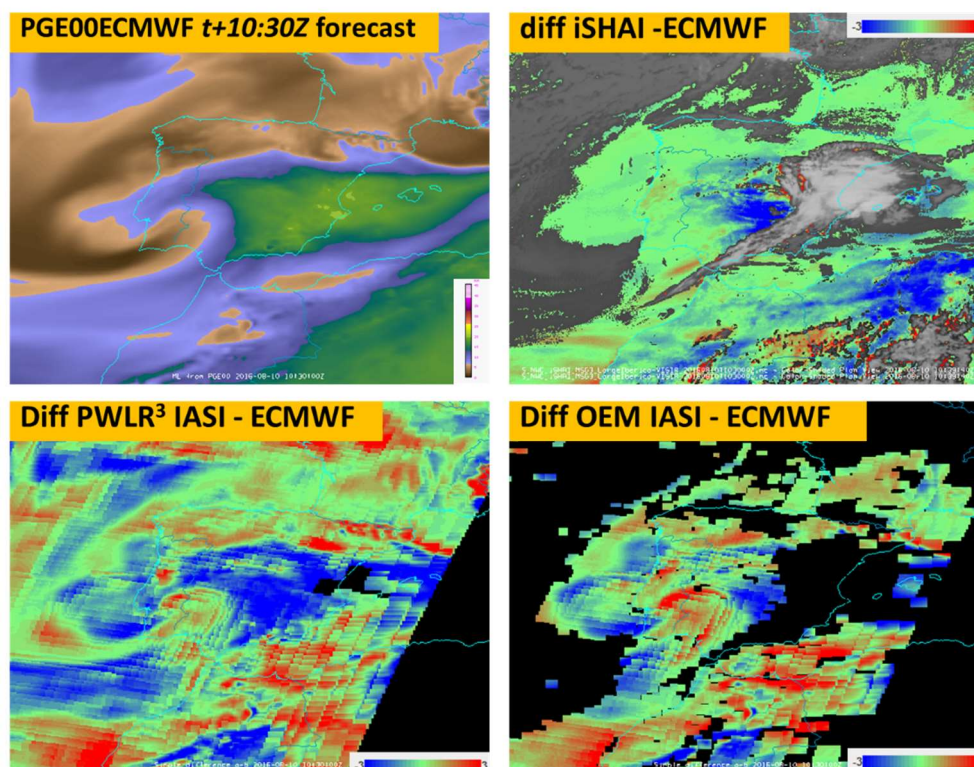



Figure 11: (top left) ML ECMWF t+10:30Z. Difference with ECMWF (top right) MSG iSHAI 10:30Z (bottom left) ES PWLR³ IASI L2 (bottom right) ES OEM IASI L2. 10th August 2016.

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3.2.1 Comparison with Sentinel missions products

As in Sentinel missions there are some products equivalents to some nowcasting parameters but estimated with higher spatial resolution and using as input other spectral ranges, there were interest in to create some process that allowed one intercomparison of both. The first that it is needed is a reader software; as Sentinel files are also netCDF files then it was created a prototype using as basis the software available for IASI netCDF files described in Section 3.1. Other of the functions needed is a remapping algorithm; instead to look for external software or tools it has been made some remapping tests applying the proposed remapping algorithm to some products from the Sentinels satellites. And last by not least the writing on netCDF compatible McIDAS-V allowed to make the intercomparison in the same projection and using the same colour palettes. These activities have been done also to explore and to create the way for using NWC SAF as an integration tool and for the possibility also to use for generation of improved training and validation dataset. In this subsection the early reprojection examples are shown; in CDOP-4 it will be done more. Also this approach could be used with NOAA or other 3rd party satellites products.

The examples of products from Sentinel-5P TROPOMI are shown in Subsection 3.2.1.1 for Total Ozone (TOZ) and Subsection 3.2.1.1 for NO₂. The example for Sentinel-3 IWV from it is shown in Subsection 3.2.1.1.

3.2.1.1 Comparison of Sentinel-5P and IASI TOZ with MSG iSHAI and ECMWF TOZ

As continuation of the studies for the proposed blended airmass RGB (see [RD.1] Section 4.1) it was made for the case study of the 8th July 2019 the intercomparison of iSHAI TOZ with MSG RGBs, EUMETSAT IASI L2 TOZ, ECMWF TOZ and Sentinel-5P TROPOMI TOZ.

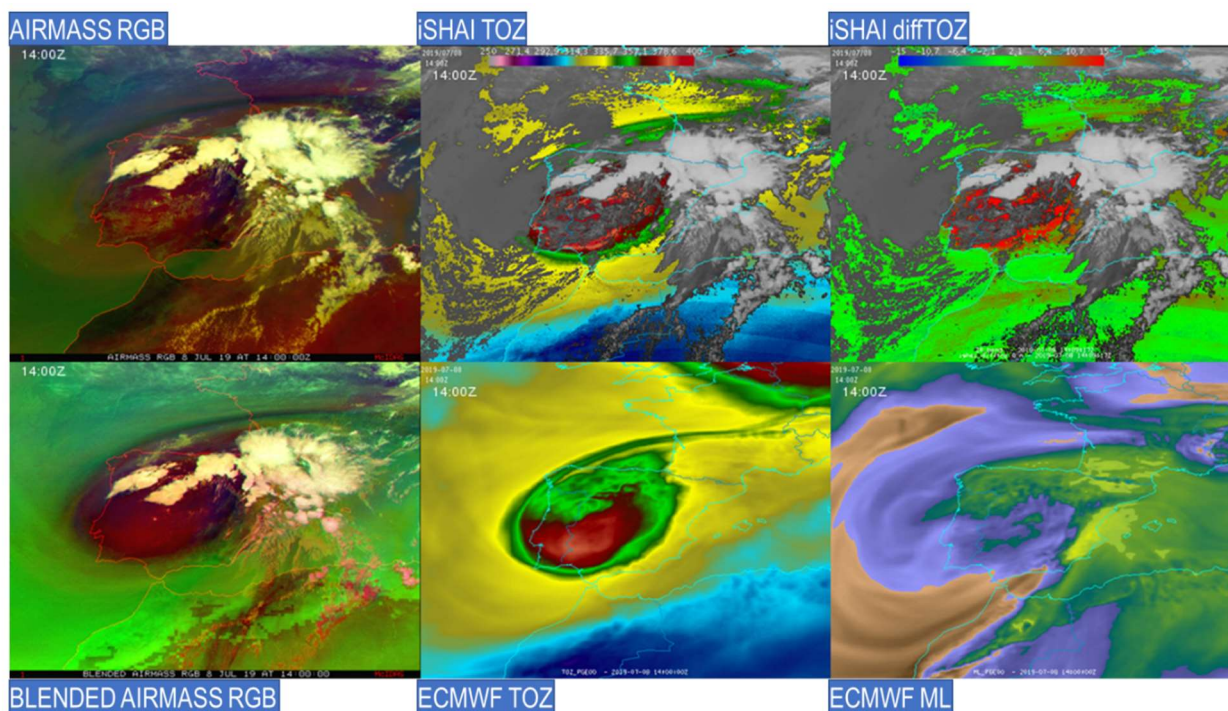


Figure 12: (top left) MSG airmass RGB. (bottom left) proposed blended MSG airmass RGB. (top centre) MSG iSHAI TOZ. (bottom centre) ECMWF TOZ $t+14$ interpolated using PGE00. (top right) MSG iSHAI difference TOZ with ECMWF. (bottom right) ECMWF ML $t+14$ interpolated using PGE00. Case study Tafalla (Navarra, Spain) 8th July 2019 at 14:00Z.

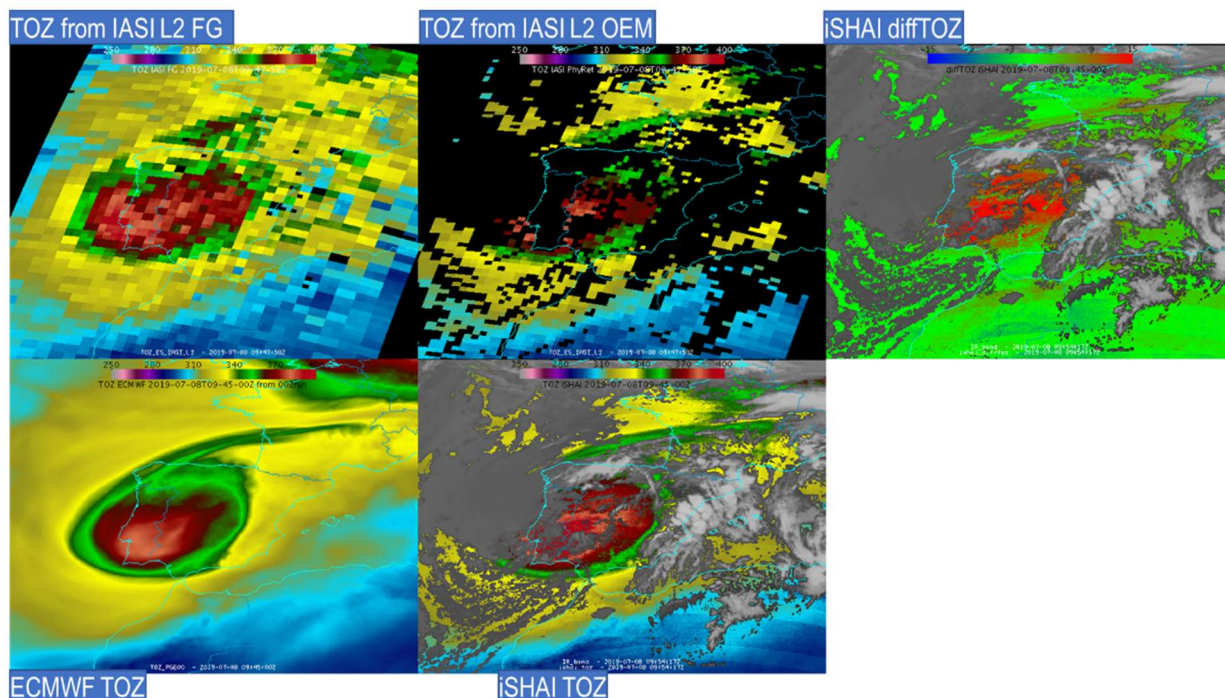


Figure 13: (top left) IASI L2 FG (PWLR³) TOZ. (bottom left) ECMWF TOZ $t+9:45$ interpolated using PGE00. (top centre) IASI L2 Optimal Estimation TOZ. (bottom centre) MSG iSHAI TOZ. (top right) MSG iSHAI difference TOZ with ECMWF. Case study Tafalla 8th July 2019 at 9:45Z.

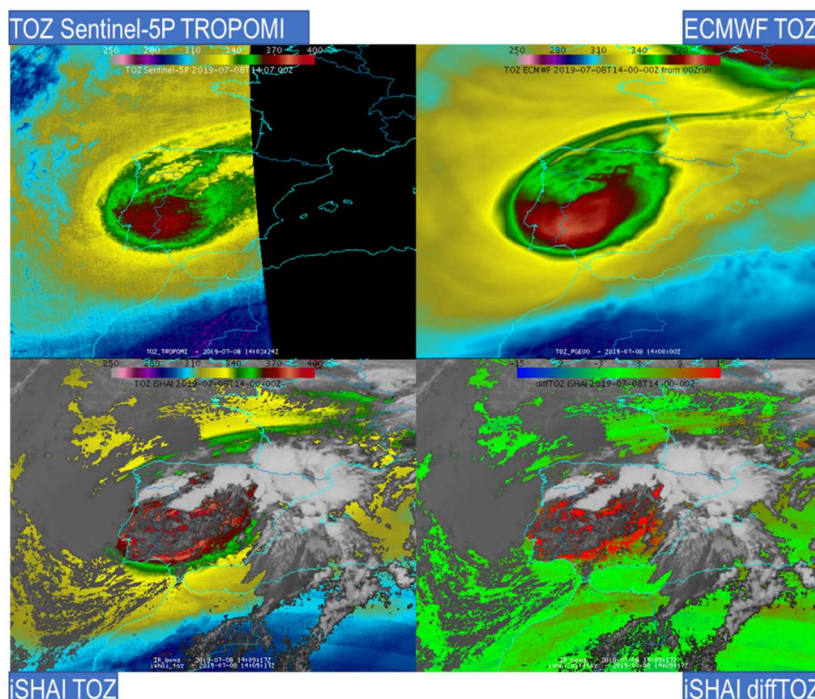



Figure 14: (top left) Sentinel-5P TROPOMI TOZ. (top right) ECMWF TOZ $t+14:00Z$ interpolated using PGE00. (bottom left) MSG iSHAI TOZ. (top left) MSG iSHAI difference TOZ with ECMWF. Case study Tafalla 8th July 2019 at 14:00Z.

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In the evening of the 8th July 2019 severe storms were triggered in Navarra (Tafalla flash flood) due to the arrival of a cold core in upper levels. This cold core in upper levels in upper levels can be seen in the Figure 12 several hours before.


It can be seen in Figure 12 (top left) that in the MSG airmass RGB it is hard to distinguish the reddish pixels of the cold core region with high TOZ values versus the reddish pixels due to hot surface pixels usual in summertime in the Iberian Peninsula. But in the Figure 12 (bottom left) with the proposed blended airmass RGB (Martinez 2018a) it is very clear the area of reddish pixels and this reddish region agrees with high values region on the forecasted ECMWF TOZ (bottom centre) as proxy of stratospheric cold air intrusion. In the proposed blended airmass RGB (Martinez 2018a or [RD.1]), it is used as green component a formula with the difference between the BTs in the IR9.7 channel of real BTs and BT RTTOV (calculated with a mean ozone profile) and corrected with the difference between the BTs in the IR10.8 channel of real and synthetic RTTOV (calculated with a mean ozone profile); see [RD.1] Section 4.1 for more details. The MSG iSHAI TOZ (top centre) also confirm this. In the Figure 12 the MSG iSHAI difference TOZ product (top right) the reddish colour pixels provides an advice that the values of TOZ are underestimated in the ECMWF TOZ; this could be understood that the stratospheric cold air intrusion is stronger than forecasted.

To try to get other independent estimation it was started the download of the IASI L2 from EUMETSAT UMARF and it was made adaptation of the remapping to also ozone profiles and the calculation of the TOZ parameter. After reading and apply the remapping to same NWCSAF region that MSG iSHAI and PGE00 ECMWF they were used in McIDAS-V tool. The intercomparison of the TOZ from IASI with ECMWF TOZ and MSG iSHAI TOZ can be seen in Figure 13 for the slot nearest to the time of IASI orbit. The spatial pattern of the TOZ fields from IASI L2 (PWLR³ FG and Optimal Estimation), ECMWF and iSHAI agrees but the values differs making difficult to get some definitive conclusion about the difference iSHAI TOZ field. The 3D ozone arrays from ECMWF, MSG iSHAI algorithm and IASI are also available and could be explored interactively with the McIDAS-V; the discrepancies in the form of the three ozone profiles on an early subjective inspection suggest that difference iSHAI TOZ likely confirm the underestimation on ECMWF TOZ in this area but perhaps due to use only an IR channel the degree of the underestimation is overvalued.

In an attempt to try to get other external referee it was started the download of Sentinel-5P TROPOMI TOZ files from the Copernicus Hub. After reading and apply the remapping to same NWCSAF region that MSG iSHAI and PGE00 ECMWF they were used in McIDAS-V tool. The intercomparison of the TOZ from Sentinel-5P with ECMWF TOZ and MSG iSHAI TOZ can be seen in Figure 14 for the slot nearest to the time of Sentinel-5P orbit. The spatial pattern of the TOZ fields agrees but unfortunately, again, the values between ECMWF TOZ and Sentinel-5P TROPOMI TOZ differ and in a different way than the values of ECMWF TOZ and IASI TOZ, so getting a conclusion is very difficult.

In the three Figures the agreement in localization of the cold core on upper levels using as proxy the TOZ field is clear. In the loop of the 24 hours every 15 minutes of RGBs, MSG iSHAI and PGE00 ECMWF fields it can be seen clearly the path followed and that the proposed blended airmass RGB works well but more time and tests are needed. Here it has been shown only as a proof of the possibilities of the generalization of remapping and intercomparison using common tools.

The investigation of the differences of IASI TOZ, MSG iSHAI TOZ and Sentinel-5P TROPOMI TOZ need more tests and they will be made in CDOP-4. When MTG-S be launched it will be the opportunity

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to repeat more similar tests using product from ECMWF, MTG-I/FCI, MTG-S/IRS and MTG-S/Sentinel-4. Thus, in future geo imager and sounder products loops could be used as a glue for the intercomparison of products from different times for polar orbit satellites.

This case study was used in October 2019 in the Valencia NWCSAF aeronautical test bed.

3.2.1.2 Remapping and combination of Sentinel-5P NO₂

During 2020 hard Covid lockdown the proposed remapping software was also adapted for the use of the Copernicus Sentinel-5P TROPOMI NO₂ estimations to estimate the reduction in contamination in Spain.

In Figure 15 it can be seen that are needed several Sentinel-5P TROPOMI NO₂ files from several consecutive orbits to cover a region like the Iberian Peninsula; also since a single day estimations are noisy it is better to combine several days. As in case of future EUMETSAT IRS L2 also the longitude and latitude arrays are included in the Copernicus Sentinel-5P netCDF-4 files.

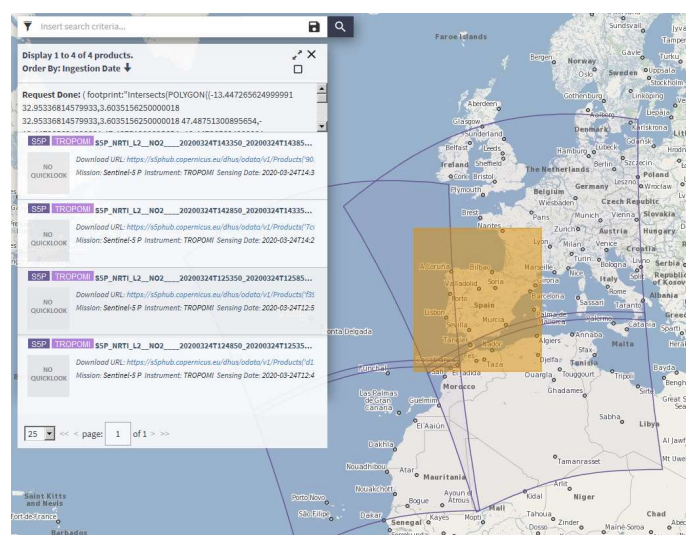


Figure 15: need of several Sentinel-5P TROPOMI NO₂ files from several consecutive orbits to cover a region like the Iberian Peninsula.

Once the S5P NO₂ estimations are read from the files download from the Copernicus hub, the array with the longitude, latitude and NO₂ estimations are written in McIDAS-V compatible remapped to the NWCSAF region shown in Figure 16 defined in MSG/SEVIRI grid. The first intention it was to add the flag on NO₂ estimations and compare with clouds from the NWCSAF operation chain but due to the need to provide a fast test it was delay for further tests.

In order to provide an image without holes the flag quality was not used and instead it has been used the Sentinel-5P TROPOMI NO₂ estimations for a period before and in the hard Covid-19 lockdown in March 2020 to show the reduction in the principal cities of the Iberian Peninsula.

Thus, all the remapped NO₂ estimations for all the files covering a period were read and calculate the mean value. In the comparison on the value of NO₂ estimations before and during the lockdown it can be seen a reduction in Madrid, Lisbon, Oporto, Barcelona, etc. during the hard Covid lockdown.

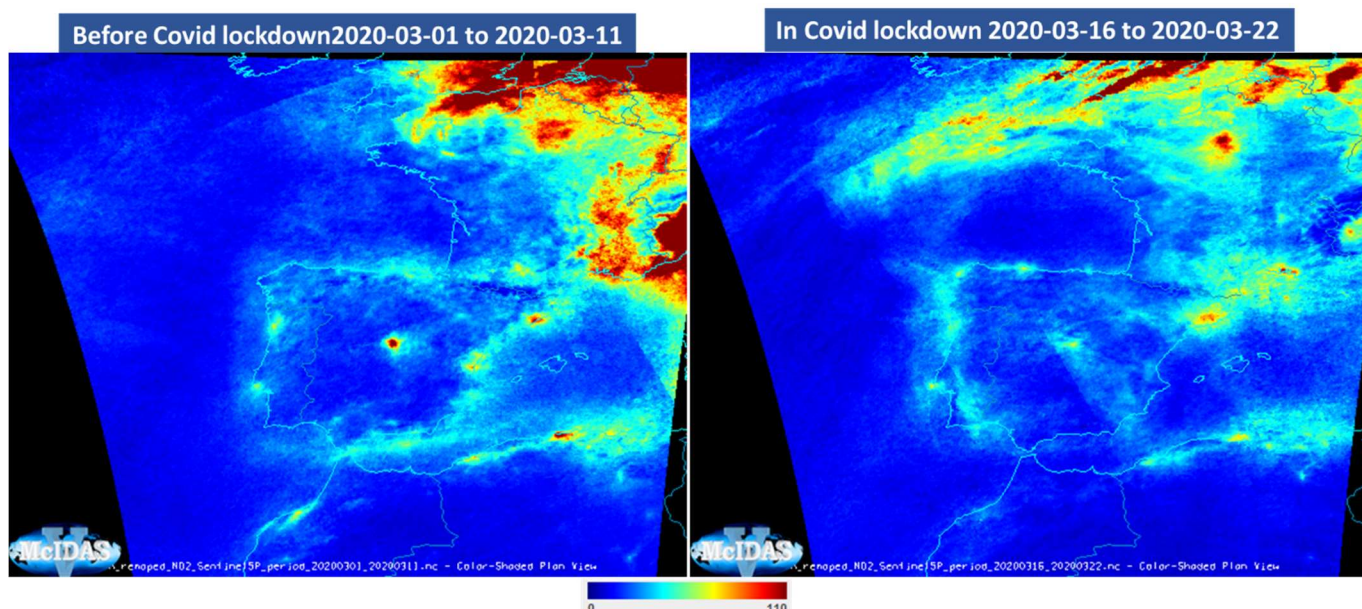


Figure 16: comparison on the value of Sentinel-5P TROPOMI NO₂ estimations before and during the hard March 2020 Covid lockdown.

But the important for this Report is the demonstration that due the fields are in a common NWCSAF region on a GEO grid the software could be adapted for the comparison of MTG L1 and L2 with other satellite missions or data sources.

3.2.1.3 Comparison of iSHAI and ECMWF TPW with OLCI Sentinel-3 IWV using inverse remapping to Sentinel-3 orbits.

The OLCI instrument on board Sentinel-3 satellites has several channels in 0.9 μm region that allows to estimate the Integrated Water Vapour (IWV) with very high spatial resolution (300 m). Since this estimation (from visible channels) could be complementary to the iSHAI estimation (from IR channels) and with higher spatial resolution it is interesting to get a comparison of the fields. Also in MTG-I/FCI there is a visible channel in the 0.9 μm region that could be used to get an estimation of IWV field for which it has been made some early tests using synthetic MTG-I/FCI data; see [RD.1] Section 4.2. For these reasons it is interesting to get a comparison of the fields after remapping to a common grid. Since the spatial resolution of Sentinel3/OLCI IWV (300 m) is much better than the MSG/SEVIRI iSHAI TPW (3 km in nadir) the natural choice is the remapping from the coarse MSG/SEVIRI resolution to narrower OLCI resolution.

Thus, in this subsection it is shown how the proposed remapping algorithm could be modified to make also the remapping in the opposite direction. So, instead to make the reprojection to a geostationary grid it is made the reprojection of the fields from the geostationary grid to the set of pixels in the polar satellite files.

In the Figure 17 it is shown the example of remapping of TPW fields from iSHAI and PGE00 ECMWF to the position of the pixels of a concatenation of two Sentinel-3/OLCI IWV files. The Sentinel-3/OLCI IWV netCDF-4 files together the longitude and latitude netCDF-4 files were downloaded from EUMETSAT UMARF and it is created a directory for every Sentinel-3 granule. As example of the

great spatial resolution it has been made a zoom of a small region near the Sistema Central in Figure 18; it can be seen also the differences in clouds (non-processed) pixels.

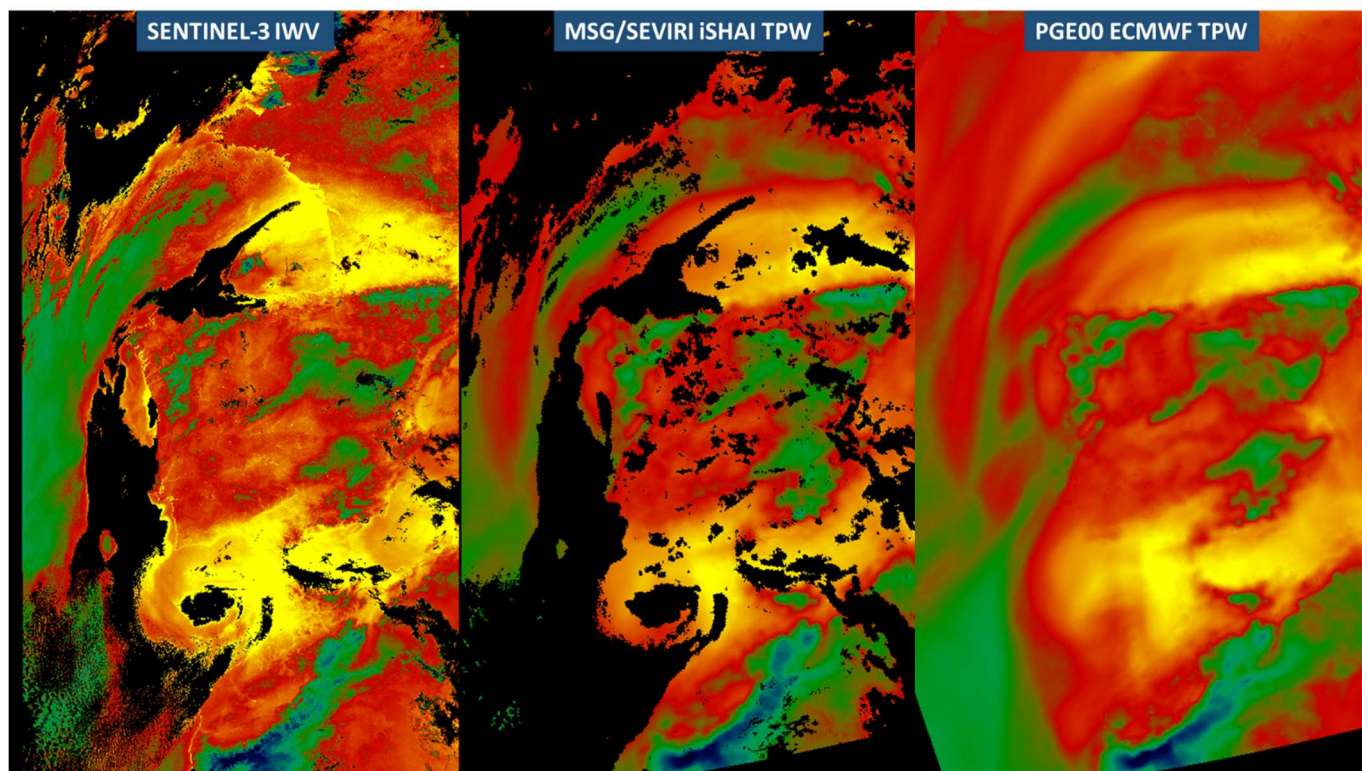


Figure 17: Comparison of (left) IWV OLCI Sentinel-3, (centre) MSG/SEVIRI iSHAI TPW, (right) ECMWF TPW using PGE00 for the interpolation to $t+10:30$. iSHAI TPW and ECMWF TPW have been remapped to OLCI Sentinel-3 positions. Case study 22nd July 2019 around 10:30Z.

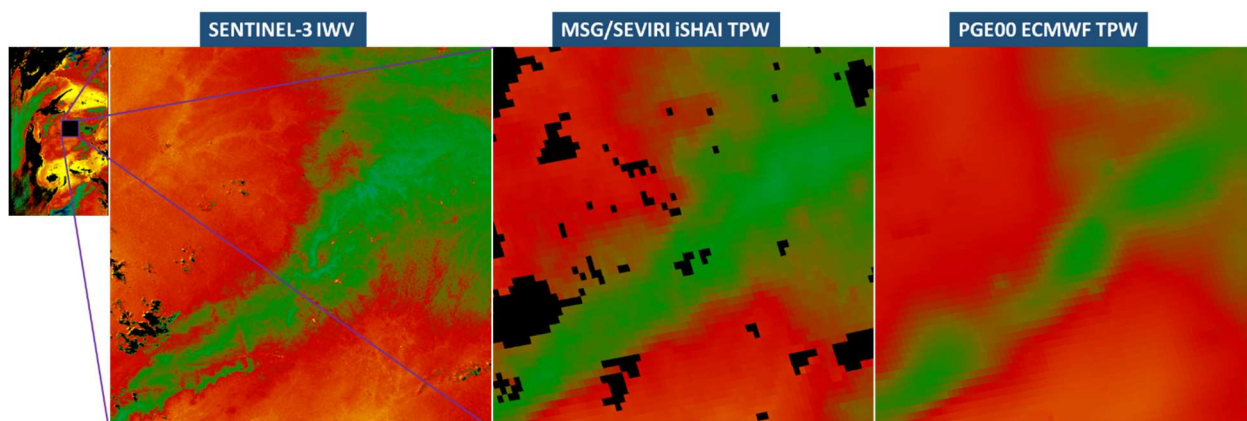



Figure 18: Zoom of fields on Figure 17. Comparison of (left) IWV OLCI Sentinel-3, (centre) MSG/SEVIRI iSHAI TPW, (right) ECMWF TPW using PGE00 for the interpolation to $t+10:30$. iSHAI TPW and ECMWF TPW have been remapped to OLCI Sentinel-3 positions. Case study 22nd July 2019 around 10:30Z.

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The modification of the remapping to make the remapping from MSG grid to the OLCI grid is easy to make:

- Read the (longitude, latitude) for every pixel in OLCI Sentinel-3 longitude and latitude arrays.
 - Using the (longitude, latitude) in the geostationary function xy2ll get (column, line) in the geostationary grid projection.
 - Using the positions and dimensions of NWCSAF region convert to (i, j) in the NWCSAF region.
 - Determine if the position (i, j) is inside of the NWCSAF region.
 - If inside NWCSAF region use the value(i, j) in case use nearest neighbor interpolation. Or use (i, j) as initial position for other kind of interpolation.
- Write the resulting interpolated matrix in OLCI Sentinel-3 grid on a file.
- Then, the two files are read and concatenated in one array for display.

These images were prepared for NWCSAF 2020 Users' Workshop (10-12 March 2020) but due to the complications in that Workshop (few days before the hard March 2020 Covid lockdown) and the uncertainties on the IWV concerning the COWa (see [link](#)) issue it was not shown in the presentation.

As summary, the main advantage is that the developed software is available and new tests with new Sentinel-3/OLCI IWV versions be will repeated in CDOP-4.

3.3 PROPOSAL OF sSHAI_ES SERVICE.


In the CDOP-3 and CDOP-4 proposals the development of a service for the support of the MTG-S/IRS L2 files disseminated by EUMETSAT Secretariat has been included. It was proposed for this service the name **sSHAI_ES**: sounder SHAI from Eumetsat Secretariat (ES) MTG-S/IRS L2. It will generate MTG-S/IRS L2 fields remapped to NWC SAF region MTG-S/IRS L2 for a set of configurable IRS L2 levels. EUMETSAT will disseminate IRS L2 products by EUMETCast on hybrid levels in 160x160 pixels dwell files.

The dissemination on dwell by dwell files will create a puzzle or tile effect; then it is convenient to have some software for combination and reprojection of 2D and 3D fields from dwells to user defined regions on a fixed (by default geostationary) grid.

Since 137 hybrid levels are hard to manage by the forecasters, then the optimal is interpolate them to users fixed pressure levels. It is also usual calculation of nowcasting parameters (TPW, LPW and Instability indices) from profiles; if they are not calculated centrally by EUMETSAT and disseminated (due to the bandwidth constraints) it is convenient to provide the calculation of nowcasting parameters (also it could be studied the calculation of additional ones by the users).


Taking into account these facts the development of the software for MTG-S/IRS L2 service will be made with the following components:

- Several MTG-S/IRS dwell files will be usually needed for covering a user configurable region of interest. Search between the set of ES MTG/IRS L2 dwell files received via EUMETCast the ones needed to cover the configurable user NWCSAF region on MTG-I/FCI grid.
- Make on every needed dwell file:

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- Read variables in ES IRS L2 files. It will be used netCDF or HDF-5 API.
- After reading of the hybrid profiles, it is made the interpolation/extrapolation to a configurable set of user predefined pressure levels. As an example in iSHAI it is used the 54 RTTOV pressure levels (used in iSHAI optional binary files). Since usually very high levels are not needed by most of nowcasting users, it can be truncated the vertical extension of the profiles to the user selection ones; this process will make a reduction on the size. As example instead of q profiles with 137 hybrid levels it would be generated an interpolated/extrapolated q profile from 200 hPa to 1000 hPa every 50 hPa.
 - It will be configurable the option to activate the extrapolation below surface pressure. In case of activation, the extrapolation procedure used in iSHAI for extrapolation below surface for ECMWF profiles on hybrid levels will be used.
- Calculation of several nowcasting parameters (TPW, LPW and instability indices) will be made also if needed. EUMETSAT has changed several times of opinion about the centralized calculation and dissemination by EUMETCast of this nowcasting parameters; due to bandwidth constraint just few of them could be disseminated. But in users' side the software could be update to calculate all the parameters needed by users. Thus, if the nowcasting interest parameters ((TPW, LPW and stability indices, etc.) are not included between the disseminated fields, then they will be calculated. By default the same NWCSAF parameters that the calculated in FCI iSHAI will be calculated.
 - Also in this step, other user configurable options as calculation of relative humidity and/or dew point profiles could be added.
 - It could be possible to add the calculation of other configurable user's choices; as example, potential equivalent temperature, normalized sigma T and q profiles, etc.; see examples in Martinez presentations.
- Then, it will be made the reprojection and combination of the fields above from the needed dwells files to user defined NWC SAF regions on to MTG-I/FCI projection (geostationary grid). This is needed because the disseminated EUMETSAT dwell files are not reprojected to a geostationary common grid and just latitude and longitude matrices are included in the dwell files. In the process it will be taking into account in the combination and reprojection of the dwell several open issues as: order of the arrays due to flip yaw maneuvers on MTG-S satellite, the performances of individual detectors, the slant perspectives, the overlapping pixels in dwell borders, etc.
- It could be added some other fields. In iSHAI files from geo imagers, it is added one configurable IR image because on displays it is better to overlap a cloud image on cloudy or non-processed pixels. It could be configured to use one IRS L1 image or one FCI L1 image.
- Finally the fields on NWC SAF regions in MTG-I/FCI projection will be written in netCDF files. The netCDF format will have a design as much compatible as possible with standard meteorological tools. As example, it will be tested to be compatible McIDAS-V.

The output of the sSHAI ES service will be a netCDF file for a configurable NWCSAF region with a combination of 3D and 2D fields. As 3D fields the file will contain as example the profiles of temperature, specific humidity and ozone on a configurable set of fixed pressure levels at the spatial resolution of MTG-I/FCI 2x2 km or at the half resolution (4x4 km) FCI grid. As 2D fields the file will contain the skin temperature, surface pressure (provided by the EUMETSAT Secretariat L2 products file to reconstruct the hybrid pressure levels), ancillary fields (longitude, latitude, orography, etc) and some parameters of nowcasting interest calculated from the temperature, humidity and ozone profiles.

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These remapped IRS L2 fields could be used later for:

- ✓ Display by users using meteorological tools. Thus, users could make the automatic generation of IRS L2 imagery related products or to use with interactive tools (as McIDAS-V).
- ✓ The fields remapped to NWCSAF regions could be used as input on locally generation of NWCSAF MTG-I/FCI or MTG-S/IRS products or other user's products. Fields as IRS L2 SKT or IRS L2 emissivity fields could be very useful to improve the MTG-I/FCI product in future versions. This way a synergetic use of the MTG mission could be get.
- ✓ It could be used for comparison to other similar products over the same regions as MTG/FCI NWCSAF products or NWP fields. As example comparison of instability indices or precipitable water fields from MTG FCI vs MTG IRS ones and versus NWP ones
- ✓ It could be used for generation of training and validation datasets.

3.4 GENERATION OF TRAINING AND VALIDATION DATASETS

When the CDOP-3 proposal was written one of the task in WP 2630 was to create a collocated dataset with IASI L1 spectra, IASI L2 retrieved profiles, NWCSAF SEVIRI outputs and ECMWF profiles. This dataset would be later used to make a comparison of the performance from iSHAI and IASI L2 outputs with other truth than radiosounding or NWP. If successful generation of the dataset, a secondary objective was the generation of one training and validation dataset for the different SHAI products.

One of the ways proposed for the generation was the participation on "EUMETSAT MTG-IRS NRT Demonstration Project" but as it has been commented in Section 3.1.1 it was cancelled the second phase.


As it shown in [RD.1] and [RD.2], in CDOP-3 the advances realized in the improvement of the AEMET PGE00 tools has allowed the generation of synthetic datasets that it has been supersede the task aimed in the proposed WP. The proposal to add IASI L2 parameters to the training and validation dataset was made thinking in to use them as a proxy of "truth" parameters for validation of imager iSHAI algorithm or IRS algorithm. But in synthetic dataset it can be used as "truth" the input profiles to the radiative transfer model.

Thus, the availability of the synthetic datasets and the delay in MTG-S launch has caused the superseding of this task by the moment for the use of the synthetic datasets. The PGE00* tools could also be used later as basis for a better generation of the proposed addition of IASI L1 and L2 to the training and validation datasets starting on commissioning phase of MTG.

3.4.1 Introduction to PGE00

A complete introduction to iSHAI and PGE00 tools is available in Chapter 2 of [RD.1] and [RD.2]. As it shown in [RD.1] and [RD.2], some of the activities has been based in the evolution of the PGE00* tools; they were used originally for validation and training of iSHAI algorithm and for the bias BT correction in NWC SAF GEO software packages. In this Section the PGE00* tools are only briefly introduced with the objective to add some notes related to 4D NWP interpolation not commented in [RD.1] and [RD.2].

In Figure 2 of [RD.1] it can be seen that one of the steps in iSHAI algorithm is the 4D interpolation from a background NWP to get collocated in time and space profiles with the satellite data. As in iSHAI this step is only made in the clear pixels (or FORs) it was created since many year ago one ad hoc tool, called PGE00, which made this process in all pixels. In the origin, PGE00 sources were a

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copy of the iSHAI (named PGE13 at this moment) sources retaining only the 4D interpolation step and suppressing the use of the Cloud Mask (CMa) as input in order to make the 4D interpolation in all the pixels. As there are not need to use satellite data and CMa as inputs it could be executed before the arrival of satellite data and by this reason it was named PGE00.

Later it was added to PGE00 the functions available on iSHAI (named PGE13 at this moment) to calculate also synthetic RTTOV BTs. Thus, PGE00* programs can be used as:

- NWP 4D (pressure, time, longitude, latitude) interpolator of NWP GRIB files to satellite positions
- RTTOV BTs simulator for bias BT correction, iSHAI validation and testing, etc

In this document the main interest from PGE00* functions are the related to the 4D interpolation of the NWP models to satellite. More specifically the 4D interpolation made from ECMWF on hybrid levels to satellite pixels on a fixed set of pressure levels.

One of the key parts in PGE00* programs is the **4D interpolation of the NWP models (ECMWF as example) to satellite positions and time**

- **The 4D interpolation (p, time, lon, lat)** get vertical, time and spatially collocated NWP forecast temperature, moisture, ozone, cc, etc. profiles at the time and position of the satellite pixels (*by default at the 54 RTTOV pressure levels*).
- ECMWF GRIB files on hybrid levels or Harmonie GRIB files complemented with ECMWF on regular representation (equidistant lon-lat) have been also used as inputs.
- The 4D-Interpolation is made in several consecutive steps:
 - Vertical interpolation: the profiles from NWP levels are interpolated or extrapolated to a configurable set of pressure levels; by default to the 54 (or 101) RTTOV pressure levels. It can made also from profiles on hybrid levels.
 - Temporal interpolation: from previous and next GRIB file to date and time of the slot
 - Spatial interpolation: bilinear interpolation to satellite coordinates
- Since the lowest RTTOV pressure levels could have values greater than the lowest hybrid level at Psfc (especially on mountains pixels) **it has been implemented in PGE00 programs one extrapolation process based in the one made by ECMWF**. First, it is made the extrapolation of the T profile (starting at the RTTOV level just above of Psfc using formulas described in the ECMWF) and then it is extrapolated the q profile maintaining the relative humidity at the surface pressure level. *This allows get fields as 1000 hPa temperature in all pixels.*
- **In the case of HYB mode all the NWP process is made inside the iSHAI or PGE00 codes.** PGE00 programs open directly the **previous** and **next** (relative to the time of the satellite image) ECMWF GRIB files on hybrid levels, make the vertical interpolation on ECMWF position to the configurable set of pressure levels, **make the temporal interpolation to the date+time of the image** and finally make the bilinear spatial interpolation just over the processed pixel (or FOR). See Figure 19.

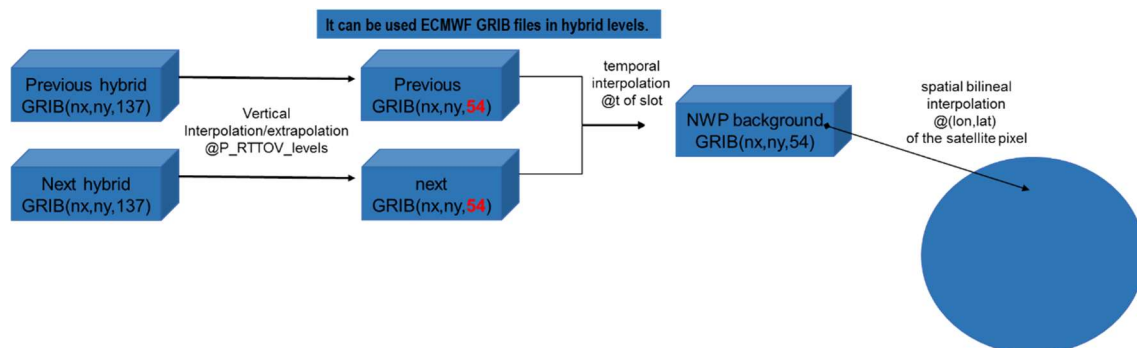


Figure 19: scheme of the 4D interpolation in the case of ECMWF GRIB files on hybrid levels.

PGE00* programs are also highly modular and configurable. The main PGE00 configurable options and parameters are:

- ✓ The window size for processing in boxes of **M x N** pixels (*default 3 x 3*).
- ✓ Optional writing for all the pixels or just at clear pixels or just on a set of pixels.
- ✓ Activation of BTs calculation also for the configured satellite.
- ✓ TOZ calculation: if GRIB files have ozone profile could be activated to make the 4D interpolation of ozone profile and to use in the RTTOV calculation.
- ✓ **The change from mode P to mode Hybrid is made changing in the iSHAI or PGE00 configuration file the keyword *NWP_EXEC_MODE* from P to HYB.**
- ✓ Activation of optional writing of temperature, specific humidity and ozone profile and skin temperature at clear processed Fields of Regards (**M x N** pixels) or for all pixels.

It is used a PGE00 Model Configuration File. All these options are activated through editing the PGE00 Model Configuration File (extension .cfm). In the PGE00* execution the third parameter is an ASCII file with all the processing options. See in more details [RD.1].

All the PGE00 programs are written in C and Fortran-90 (but the core of the process is Fortran90 as in the RTTOV sources).


All of these facts could be used as basis for routines in the development of the sSHAI_ES service.

3.4.2 Use of PGE00* for synthetic 4D datacubes generation.

The initial PGE00 programs was only able to calculate synthetic RTTOV BTs on clear air conditions. The actual versions of GEO-PGE00-VISIR and GEO-PGE00-hyper make the simulation of clouds using the clouds parameters profiles in the simulations. As can be seen in [RD.1] and [RD.2] These GEO-PGE00-* programs are important because they are the first able to generate the synthetic data on the future MTG-I/FCI grid.

GEO-PGE00-VISIR allows to simulate GEO imager instruments on NWCSAF regions using 4D interpolation from NWP GRIB files. *GEO-PGE00-hyper* allows to simulate sounder instruments on NWCSAF regions using 4D interpolation from NWP GRIB files. *GEO-PGE00-hyper* was used for the generation of first high quality synthetic clear and cloudy BTs of IASI and IRS.

As can be seen in [RD.1] and [RD.2], variants of these PGE00* tools were used for the generation of high spatial resolution synthetic datasets. In the case of PGE00* tools used with Harmonie

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complemented with ozone profiles from ECMWF model it has been used some of the remapping function developed for the remapping of IASI or IRS L2 products.

As the actual versions of PGE00* tools use RTTOV-13.0, that it is the first RTTOV version with coefficients for the final IRS spectral grid, these 4D datacubes are the first scientifically realistic synthetic datasets with collocated MSG/SEVIRI, MTG-I/FCI, MTG-S/IRS and IASI synthetic radiances on MTG-I/FCI grid. It can be seen examples of 24 hours loops from these 4D datacubes in Martinez 2020 presentations.

The 4D datacube for case study 1st May 2019 it contains 24 hours synthetic data with collocated on MTG-I/FCI grid:

- ✓ MTG-I/FCI: synthetic radiances for clear and cloud conditions every 10 minutes on 1x1 and 2x2 MTG-I/FCI grids.
- ✓ MTG-S/IRS: synthetic BTs for clear and cloud conditions every 30 minutes on 2x2 MTG-I/FCI grid.
- ✓ IASI: synthetic BTs for clear and cloud conditions every 30 minutes on 2x2 MTG-I/FCI grid.
- ✓ MSG/SEVIRI: synthetic radiances for clear and cloud conditions every 10 minutes on 1x1 and 2x2 MTG-I/FCI grids. Also synthetic radiances for clear and cloud conditions every 15 minutes on 1x1 MSG/SEVIRI grid; real MSG/SEVIRI radiances are also available.
- ✓ The 4D interpolated profiles from NWP at the 54 RTTOV for T/q/ozone/cc/clwc/cwic/u/v every 10 minutes on the 1x1 MTG-I/FCI grid. Also the same profiles every 30 minutes on the 2x2 MTG-I/FCI grid. Surface fields from NWP: P_{sfc} , Skin Temperature (SKT), T_{2m} , q_{2m}
- ✓ Ancillary fields: longitude, latitude, topography, sun angles and GEO satellite angles for the satellite configured in `SSAFNWC/config/sat_conf_file`


In the case of 4D datacube from Harmonie NWP model complemented with ECMWF for case studye 25th of April only for the synthetic MTG-I/FCI and MTG-S/IRS radiances are available but could be generated the MSG and IASI ones.

In summary these 24hours synthetic datasets complemented with the profiles using as input to the RTTOV model has allowed to create 4D datacubes that it far exceeds expectations with the proposed generation of collocated dataset of IASI L1 and IASI L2.

3.4.3 PGE00_1d version for generation of reference training and validation.

For calculation of new iSHAI coefficients and for validation statistics (writing of the iSHAI Validation Reports) it was started to use always a reduced PGE00 version called internally *PGE00_1d* during all NWC SAF phases.

Basically this *PGE00_1d* version is one only FORTRAN program that reads a binary file with a set of records for every pixel and generate as output the RTTOV synthetic BTs in clear air conditions. The used RTTOV functions are the same used in PGE00 and iSHAI of the same versions. The binary input file is easily written using IDL or C o FORTRAN. The output are just $N_{channels} \times N_{pixels}$ floats in a binary file. The version of *PGE00_1d* using RTTOV-13.0 developed in 2021 will be the one used initially in CDOP-4 phase. It allows to get synthetic radiances for any satellite with RTTOV coefficients for the same profile. Thus, MSG/SEVIRI, MTG-I/FCI, MTG-S/IRS and IASI synthetic radiances could be calculated.

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Together with the *PGE00_1d* program it is needed to use a reference dataset. From the beginning of CDOP-3, it was generated the 2017 training and validation dataset. The combination of the *PGE00_1d* program and the reference dataset can be used to generate synthetic datasets for two branches: one for GEO imager instruments and other for hyperspectral or sounder instruments.

It can be seen in Figure 20 that this 2017 training and validation dataset could be used also to generate synthetic datasets for both imager and sounder instruments. In the case of GEO imager instruments it has been used for the generation iSHAI coefficients and Validation Reports for version 2018*, 2021 and preliminary vMGT (for STRR reviews). In Figure 20, it is also shown that the synthetic imager and sounder datasets could be used together to explore the possibility to make one assessment of the performance of future blended FCI and IRS products.

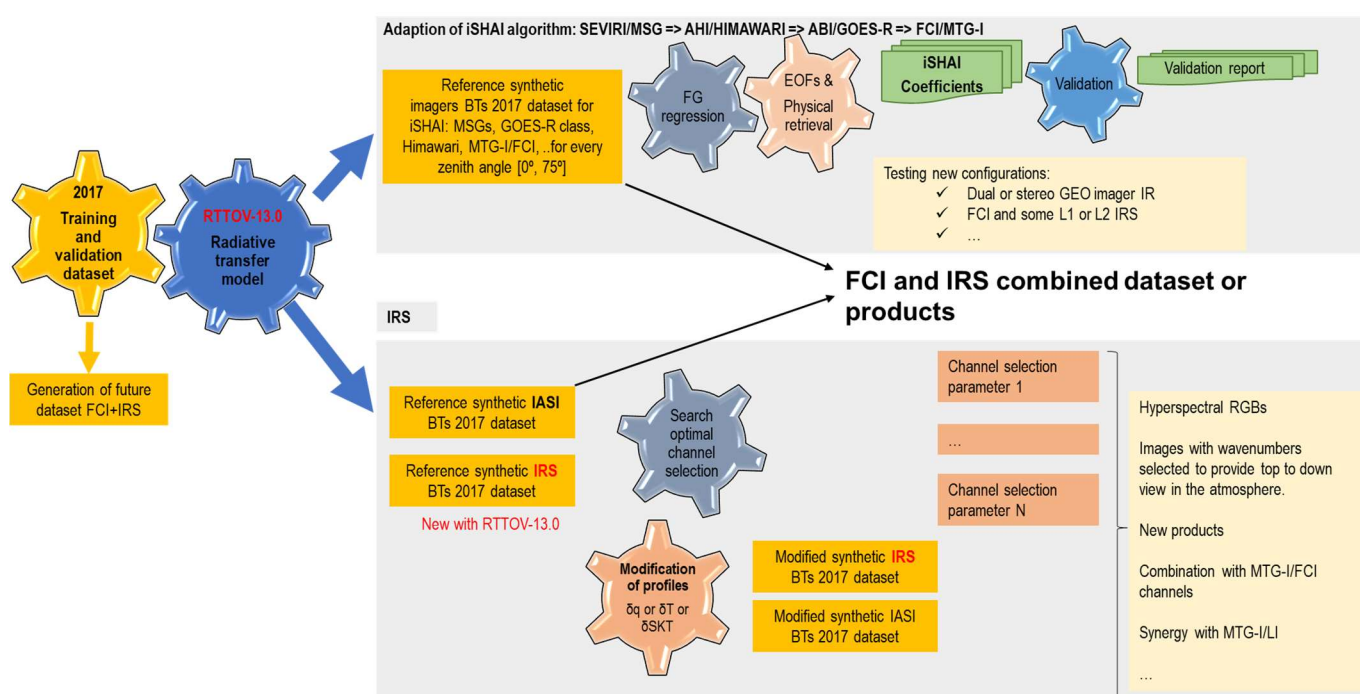



Figure 20: scheme of the *PGE00_1d* use for training and validation activities.

In CDOP-4 it could be generated more training and validation datasets, the important now is that it has been created the tools to build them. In CDOP-4 commissioning phase of MTG-S/IRS it could be incorporated real IRS and FCI data; then, the training and validation datasets combining real and synthetic data could be used for bias BT detection, tuning of coefficients, writing of validation reports, etc.

As it has been shown in this Report for several case studies it could be generated specific datacube with the addition of IASI L1 data and IASI L2 products together with other satellite missions (Sentinels or 3rd party satellites).

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4 CONCLUSIONS, SUMMARY AND FUTURE ACTIVITIES

The tests, studies and ideas described in this Report will help to implement the generation of NWC SAF products and services for MTG-S/IRS L1 and L2. These studies are also valuable to anticipate the new ways that whole set of MTG L1 data and L2 products could be used in MTG era for nowcasting. All these experiences will be used as basis for one operational service of L2 products received from EUMETCast and for the generation to the validation and training dataset of MTG-I/FCI and MTG-S/IRS L1 and L2 products.

The NWC SAF is developing software packages that will allow to manage the data from all the three MTG instruments and to generate locally products by the users. Since NWC SAF provide software that it is installed on the users' computers there are no bandwidth constraints and the whole set could be used in combination with local NWP and data. Thus, all the synergies can be exploited.

NWC SAF will deliver an optional and complementary software package in order nowcasting users could make use of MTG-S/IRS L1 data disseminated in PC, together with EUMETSAT Secretariat IRS L2 products and locally generated NWCSAF MTG-S/IRS L2. The sSHAI_ES service will allow in Day-2 to add the EUMETSAT MTG-S/IRS L2 products to the local users' data cube.


The main lesson learned of the activities with EUMETSAT MTG-IRS NRT Demonstration Project, EUMETSAT UMARF IASI L2 and Sentinel products described in this Report is that depending on the final Level 2 format specification, the gap between user's tools and MTG-S/IRS L2 output files could be more or less large but always some kind of tools should be provided to the users. It is clear that usually L2 files are written not thinking in to be exploited directly with meteorological tools. This is another example of the need of NWC SAF software in the users' side of EUMETCAST to cover the gap between EUMETSAT disseminated files and users' needs.

Validation and training dataset generation is a continuous and important task. The participation of AEMET clear air team on EUMETSAT MTG-IRS NRT Demonstration Project did not provide an adequate validation and training dataset generation with IASI L2 but it has provided the basis of the tools to build it in future. The synthetic dataset created with PGE00* tools can be used as better option in the early stage. Some of the functions developed in these activities will be needed in CDOP-4 for generation of training and validation datasets with real data.


For the development of the operational tools for optimal reprojection and concatenation of MTG-S/IRS L2 dwells files to NWCSAF MTG-I/FCI projection it is needed that EUMESAT will provide IRS L2 test files on full disk or at least in LAC4 region for a period.

With the recent incorporation of new machines (with more memory available) and the new IDL8.8 version it will be increased the number of tests and studies that can be boarded. Also it will be tested new possibilities as the use external tools through Python interfaces. The decision of the migration from IDL to Python or Fortran/C as proxy or future NWCSAF developments will be taken later during CDOP-4 phase.

If the two software package are installed and executed in a PC or in several PCs in parallel with some synchronization of the directories. In any case it will be studied the coordination and interrelation between both NWCSAF software package instances. Although in some PGE00* tools has been used parallelization, since UNIX machines allow to launch several programs at same time it should be decided if used execution at the same time of processing programs for several dwell files at same time or to execute only a processing dwell program with parallelization (OpenMP RTTOV interface). Due the low number of threads available (4 to 10) in a normal PC machine it will be tested the optimal sequence on the reduction of time. Depending in the final performance estimations it will be studied

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the recommendation of execution of IRS package in more powerful computers with more threads available.

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