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DOCUMENT

Outcomes and Recommendations from the: *Uncertainty in Remote Sensing Workshop*

ESRIN; 24 – 25 Oct 2017

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1 SUMMARY

During 24 – 25 Oct 2017 a two days workshop was held in ESRIN with the objectives to review the state of the art on uncertainty estimation for EO remote sensing data and to collect recommendations on how to improve current theoretical approaches and foster the adoption of common best practices across the various communities.

The workshop was promoted by ESA-SPPA section, and it is part of the section's effort in the evolution of algorithm and validation methods in support to current and future ESA EO operational missions. The outcomes of the workshop will contribute to shape the strategy of ESA-SPPA section for the provision of enhanced quality information in the users' products. The long-term goal is to eventually implement the recommendations gathered during the workshop in the operational production of ESA EO data.

This document provides an overview of the main outcomes from the workshop and the recommendations and feedback gathered from the participants during the discussion session. Additional details, including presentations and notes from the discussion session can be found at the following address:

https://earth.esa.int/web/sppa/meetings-workshops/expert-meetings/workshop-on-uncertainties-in-remote-sensing

1.1 Acronyms and Abbreviations

AOT	Aerosol Optical Thickness
AVHRR	Advanced Very High Resolution Radiometer
BA	Burned Area
BOA	Bottom of Atmosphere
Cal/Val	Calibration and Validation
CCI	Climate Change Initiative
CDR	Climate Data Record
C3S	Copernicus Climate Change Service
DHP	Digital Hemispheric Photography
ECV	Essential Climate Variable
EO	Earth Observation
ESA	European Space Agency
FAPAR	Fraction of Absorbed Photosynthetically Active Radiation
FIDUCEO	Fidelity and Uncertainty in Climate data records from Earth Observations
FCDR	Fundamental Climate Data Record
FRM	Fiducial Reference Measurements
GCOS	Global Climate Observing System
GUM	Guide to the Expression of Uncertainty in Measurement
LST	Land Surface Temperature
MERIS	MEdium Resolution Imaging Spectrometer
MODIS	Moderate Resolution Imaging Spectroradiometer
MSI	Multi-Spectral Instrument on-board S2
NASA	National Aeronautical and Space Administration
NDVI	Normalized Difference Vegetation Index

NIR	Near-InfraRed
NN	Neural Network
NPL	National Physical Laboratory
OLCI	Ocean and Land Colour Instrument on board Sentinel-3
PAR	Photosynthetically Active Radiation
PDF	Portable Document Format
PROBA-V	Project for on-board Autonomy-Vegetation
QA	Quality Assessment
QA4EO	Quality Assurance Framework for Earth Observation
QA4ECV	Quality Assurance for Essential Climate Variables:
RTM	Radiative Transfer Model
SI	International System of Units
SLSTR	Sea and Land Surface Temperature Radiometer
SM	Soil Moisture
SPPA	Sensor Performances Products and Algorithm Section of ESA/EOPG
SR	Surface Reflectance
SSES	Sensor Specific Error Statistic
SST	Sea Surface Temperature
SWIR	Short-Wave InfraRed
SWE	Snow Water Equivalent
S2	Sentinel-2
S3	Sentinel-3
TCWV	Total Column Water Vapour
TIR	Thermal Infrared
TOA	Top-Of-Atmosphere
UAV	Unmanned Aerial Vehicle
VNIR	Visible and Near-InfraRed
VIIRS	Visible Infrared Imaging Radiometer Suite

1.2 References

[RD-1] QA4EO: Quality Assurance Framework for Earth Observation: http://qa4eo.org

[RD-2] Fiduceo Project: Fidelity and uncertainty in climate data records from Earth Observations. See the project website at: http://www.fiduceo.eu

[RD-3] QA4ECV: Quality Assurance for Essential Climate Variables: http://www.qa4ecv.eu

[RD-4] Theocharous, E., & Fox, N. P. (2016). Fiducial Reference Measurements for validation of Surface Temperature from Satellites (FRM4STS)-Laboratory Calibration of Participants Radiometers and Blackbodies. Protocol for the FRM4STS LCE (LCE-IP), ESA Contract No. 4000113848_15I-LG, NPL report OFE-D-90A-V1-Iss-1-Ver-1.

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[RD-7] ESA Climate Change Initiative, CCI: http://cci.esa.int

[RD-8] Copernicus Climate Change Service (C3S): https://climate.copernicus.eu

[RD-9] GUM: Guide to the Expression of Uncertainty in Measurement: https://www.bipm.org/en/publications/guides/gum.html

[RD-10] TRUTHS: Traceable Radiometry Underpinning Terrestrial- and Helio- Studies: http://www.npl.co.uk/truths/

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[RD-13] Vermote, E. F., & Kotchenova, S. (2008). Atmospheric correction for the monitoring of land surfaces. Journal of Geophysical Research: Atmospheres, 113(D23).

[RD-14] ACIX: Atmospheric Correction Inter-comparison Exercise: https://earth.esa.int/web/sppa/meetings-workshops/acix

[RD-15] Gobron, N., Pinty, B., Aussedat, O., Taberner, M., Faber, O., Mélin, F., ... & Snoeij, P. (2008). Uncertainty estimates for the FAPAR operational products derived from MERIS—Impact of top-of-atmosphere radiance uncertainties and validation with field data. Remote Sensing of Environment, 112(4), 1871-1883.

[RD-16] Enviro-Net Network lead by University of Alberta: http://www.enviro-net.org

[RD-17] GAIA-CLIM project web-site: http://www.gaia-clim.eu; The GAIA-CLIM Virtual Laboratory tool can be accessed at: http://193.40.13.83/vo-dev/index.html#/

2 INTRODUCTION

This section illustrates the motivations and objectives for organizing the Workshop on Uncertainty in Remote Sensing, which was held in ESRIN during 24 – 25 Oct 2017.

2.1 Motivations

The assessment of uncertainty for EO remote sensing data is a crucial requirement from the user community, notably in the context of climate applications, weather forecast modeling, as well as, for policy definition.

Calibration/Validation (Cal/Val) activities are essential to uncertainty estimation, by providing the reference "ground-truth" data, which is needed to estimate (or validate) the error budget associated to the remote sensing products. While this general concept is unanimously recognized, the methodologies developed are very diverse, both in terms of in-situ measurement protocols and theoretical approaches and formalism for error budget estimation.

In order to answer to the lack of harmonized procedures and considering the relevance of such topic for the user community, a number of international projects and initiatives were carried out in the recent years. Among them, the following ones are the most relevant for the scope of this document: the **QA4EO** project

[RD-1], which provided the general framework for QA of EO data, the **Fiduceo** [RD-2], and the **QA4ECV** projects [RD-3], which are addressing the needs for uncertainty estimation in the frame of Climate Data Record (CDR) generation, and the concept of **Fiducial Reference Measurement (FRM)** [RD-4], which was recently developed by the European Space Agency (ESA) and it is promoted to address the need for SI traceability and community-agreed protocols for in-situ Cal/Val measurements. A more comprehensive overview of the state-of-the art in terms of projects, methodologies and approaches for uncertainty estimation was recently published in two review papers [RD-5], [RD-6].

In this context, and with the intention to contribute to such major on-going international effort, the ESA-SPPA section in collaboration with the University of Reading and the National Physical Laboratory (NPL) organized a workshop dedicated to Uncertainty in Remote Sensing.

The ESA-SPPA section was strongly involved in most of the projects of relevance for this topic, in particular in the QA4EO and FRM activities, and it is responsible for Cal/Val and Data Quality activities in support to ESA operational and historical missions. Both NPL and University of Reading have a leading role within the Fiduceo and QA4ECV projects and contributed to several activities related to uncertainty estimation in the frame of ESA Climate Change Initiative (CCI) [RD-7] and of the Copernicus Climate Change Service (C3S) [RD-8].

2.2 Objectives

The **objectives** of the Workshop were:

- To present the state of the art for uncertainty estimation for EO remote sensing data;
- To illustrate the general theoretical framework and promote a metrological perspective;
- To foster the use of a common terminology and best practices;
- To review the various methodologies and approaches across communities;
- To identify current limitations and discuss potential evolutions in protocols and methods;
- To discuss on the validation of uncertainty estimation;
- To gather recommendations on the best strategy for providing uncertainty information to users in an operational manner;

3 WORKSHOP PROCEEDINGS

The status of uncertainty characterization in EO data was generally recognized as inadequate, since there is still a lack of clear information on the confidence and *fit-for-purpose* of EO data and this has a significant impact both on the science applications as well as on the policy making process. The current workshop should contribute in this context by identifying the areas where we need to focus more to fill this gap.

The workshop was organized around three main sessions:

- *Theoretical Framework* – An initial session, during which, key scientists from University of Reading and the National Physical Laboratory (NPL) presented the general theoretical framework and the basic terminology relevant for uncertainty estimation.
- *State of the art* – A session dedicated to examples of application of uncertainty estimation in EO remote sensing, both for Level 1 products (radiance/reflectance) and for the derived Level 2 products (the geophysical products).
- *Discussion and Recommendations* – A discussion session driven by a set of seed questions, during this session the feedback from all participants was stimulated and the most relevant answers were collected and formulated in an initial set of main recommendations to the Space Agencies.

3.1 Theoretical Framework

The theory and terminology for assessing uncertainty in EO remote sensing data was illustrated by NPL and University of Reading.

Traceability

A measurement result is defined traceable when it can be traced to a stated metrological standard (ideally SI) through an unbroken chain of calibrations, each contributing to the final measurement uncertainty. Traceability can be guaranteed in laboratory-controlled conditions, while **satellite-based systems are not (at present) fully traceable to metrological standard**, unless an in-orbit SI-traceable system is designed for the mission [RD-10]. On the other hand, traceability, as a general principle, should be applied to EO, both for ensuring rigorous error propagation through the full processing chain (QA4EO principles) and for defining more stringent requirements for the collection of in-situ validation data (FRM concept).

Uncertainty Analysis

The measurement uncertainty is a non-negative parameter characterizing the dispersion of the quantity values being attributed to a measurand (the quantity to be measured), while the error is the difference between the measured value and the *true* value of the measurand. The **Guide to the Expression of Uncertainty in Measurement (GUM)** [RD-9] provides the guidelines to rigorously assess the uncertainty of the final measurement following the traceability tree. A thorough uncertainty analysis includes the identification and categorization of all possible error sources in particular the random and systematic component as well as any correlation (spatial, temporal, spectral).

Lessons from Fiduceo

A rigorous metrological approach to uncertainty was adopted in the frame of the Fiduceo project in order to derive Fundamental Climate Data Record (FCDR) of AVHRR TOA Earth radiances for the thermal bands. The series of AVHRR sensors, which is potentially of extreme interest for climate, poses notably some major challenges in terms of long-term consistency and stability, owing to the various calibration issues documented in the literature and to the orbital drifts of the different NOAA platforms. As demonstrated within the Fiduceo project, a rigorous recalibration of the long-term data series was required in order to remove all the spurious trends and abrupt changes induced by external factors, e.g., instrument thermal evolution, orbital drift, solar contamination.

As a result of Fiduceo project a series of lessons learned were collected:

- **A metrological approach shall be applied as early as possible during the design phase of a satellite mission, this includes both the definition of the on-ground characterization measurements and the specification of the users' products;**
- **A close monitoring of the instrument performance evolution shall be carried out while in-orbit in order to correct for evolution of environmental conditions;**
- **A thorough error propagation approach shall be followed and applied, uncertainty shall be provided per-datum to the users with an adequate documentation on how to use this information;**
- **The traceability and metrological principles shall be embedded into current Space Agencies' practices on providing EO remote sensing data for both historical and future missions;**

3.2 State of the art

The session on the state-of-the-art presented some relevant examples on how uncertainty information is currently estimated by the different communities; the examples cover a wide range of applications, spanning from land, water to atmospheric domains. Highlights and recommendations are reported in the following paragraphs.

3.2.1 Level 1 products

There is an on-going effort at ESA to support the definition and provision to users of uncertainty per-pixel to be embedded into the Level 1 products (TOA radiance/reflectance). The uncertainty budget estimation for these products is often focused on the radiometric uncertainty, which is derived using a combination of on-ground characterization measurements and periodic in-flight calibration using the on-board calibration devices. Examples of uncertainty estimation for Level 1 products of S2 MSI, S3 SLSTR and S3 OLCI sensors were presented.

Sentinel-2 MSI

The **RUT (Radiometric Uncertainty Tool)** [RD-11] was developed at NPL for estimating a **per-pixel radiometric uncertainty associated to S-2 Level 1c product.** The S2 RUT is based on the definition of a radiometric model and it follows a **metrological approach** to identify all possible sources of uncertainty and estimate their contribution to the TOA reflectance by propagating their impact along the measurement equation. Despite the possibility to effectively provide an uncertainty per pixel in Level 1 data, there are still numerous **challenges to be addressed, in particular a rigorous treatment of the impact of orthorectification, resampling and the resulting interpolation errors, which introduce correlation between pixels, additional effects, which are not fully characterized, such as impact of stray-light and polarisation.** The full understanding of these error contributors requires a deep knowledge of the instrument design, e.g., the S-2 detectors module arrangement, and it is sometime hindered by a non-adequate on-ground characterization of the sensor.

Sentinel-3 SLSTR

The radiometric uncertainty estimation for S3-SLSTR was based upon the lessons learned with the design and operations of ATSR sensors. **There was historically a strong focus on uncertainty budget estimation for the ATSR family of sensors, owing to its relevance for climate applications** and the resulting stringent requirement on the its main geophysical product, the Sea Surface Temperature (SST), i.e., 0.02K accuracy and 0.02K stability per decade. These stringent requirements were driving the instrument design and the set-up of the on-ground characterization. As a result, **the SLSTR sensor has one of the most sophisticated in-flight systems for autonomous calibration,** consisting on a set of BB sources for the TIR channels, ensuring the in-flight traceability, and the VISCAL assembly for the solar channels, furthermore, an extensive pre-flight calibration campaign was carried out [RD-12]. A very detailed uncertainty budget is derived from the calibration model and propagated through the full Level 1 processing chain, following the traceability tree. On the other hand, **the current information for SLSTR Level 1 products includes the detector noise and the uncertainty estimation per band as a function of the scene temperature based on pre-flight measurements. No uncertainty information per-pixel is currently provided in SLSTR Level 1 products.**

Sentinel-3 OLCI

Similarly, for S3-OLCI there is currently no uncertainty information at pixel level. Though. a way forward was presented on how to address this need, by identifying all error contributors, characterize their uncertainty and propagate it through the full Level 1 processing chain. **Several issues need still to be investigated in detail, in particular, the impact of stray-light correction, detectors non-linearity, sun-diffuser BRDF characterization, and primary diffuser degradation modeling.** Furthermore, an investigation is on going on the possibility to adopt a similar approach, as for the S-2 RUT.

3.2.2 Level 2 Land products

The first satellite-based Level 2 products for land applications are the Bottom-Of-Atmosphere (BOA) radiance/reflectance products, often referred as Surface Reflectance (SR). The BOA products are the output of the atmospheric-correction process, consisting in the estimation and removal of the atmospheric contribution to the TOA at-sensor radiometric signal. **The error budget associated to the atmospheric correction process includes all the approximations used to simulate the inherent radiative transfer process, and the uncertainty in the estimation of the atmospheric constituents**

concentration. Typically, in the solar spectrum and for the commonly used visible spectral bands, the error budget is dominated by the uncertainty in the estimation of the aerosol and water vapour optical properties. **The** uncertainty estimation in BOA products is then propagated into the biophysical retrieval algorithms for assessing the error budget of the derived Level 2 and Level 3 products. Examples of uncertainty estimation for BOA products and derived biophysical variables were presented and discussed.

Surface Reflectances

A solid approach was developed at NASA for the estimation of the uncertainty budget in the derived SR. This approach, originally developed for MODIS, was recently extended to Landsat-8 and Sentinel-2 SR. The method allows for the assessment of the uncertainty associated with the atmospheric correction process, which is based on an empirical retrieval of AOT and on the use of the 6SV radiative transfer code [RD-13]. The validation of both AOT and surface reflectance is performed over a large set of AERONET stations globally spread to be representative of different surface and climatological conditions. In the absence of a globally representative network of in situ measurements, a “ground-truth” dataset of synthetic surface reflectances is computed over selected AERONET stations using the AOT and TCWV provided by AERONET retrievals. A protocol was developed allowing to quantitatively estimating the error budget for the obtained surface reflectance in terms of Accuracy, Precision and Uncertainty (APU). This protocol has been recently adopted in the frame of the ACIX intercomparison exercise for Sentinel-2 and Landsat-8 atmospheric correction [RD-14]. This protocol has proven to be very effective and **the use of AERONET-derived surface reflectance is a pragmatic solution to the lack of an operational extended network of in-situ surface reflectance measurements representative of different surface and environmental conditions. The importance of a detailed error budget analysis was underlined, both for improving the algorithm and for understanding and controlling the results of the validation. The final goal of the validation is to reconcile the prior estimation of the error budget with the one obtained with in-situ measurements.**

Land Surface ECVs (FAPAR, LAI, Albedo)

Uncertainty information per-pixel is currently embedded within the Sentinel-3 operational FAPAR products, based on the algorithm and methods developed at JRC for MERIS [RD-15] and further refined for OLCI. The algorithm considers only the contribution from the green elements at the time of the satellite overpass, resulting in the Green black-sky FAPAR. The error budget takes into account the retrieval uncertainties and the errors associated with approximations in the RTM simulation, under the assumption that these uncertainties are totally independent. Error propagation is used following the GUM guidelines. When validating the satellite-based estimate it is crucial to properly characterize the uncertainty associated with the in-situ measurements. **The ground-based measurements do not measure the true value of the land ECV (e.g., FAPAR, or LAI), but they infer this value from indirect measurements, in addition, in particular for FAPAR different algorithms may use different FAPAR definitions (white-sky, black sky, total or green FAPAR). Since the true value cannot be measured on-ground, JRC has developed a 3D RTM to estimate the true value of the land ECVs of interest (FAPAR, LAI, Albedo) for different biomes and canopy structure and to mimic the signal that would be measured from a satellite and from ground-based observations.** Application of this model to simulate a ground-based campaign of FAPAR measurements using Digital Hemispheric Photography (DHP) is presented. **The 3D RTM allows for the simulation of a virtual field campaign and it can be used to find the optimal sampling design (e.g., best transect) for different biomes and to ultimately infer the total error budget associated to the ground-based observations**. The importance of the FAPAR definition is finally recalled, this is crucial when validating the satellite estimate with ground-based measurements as well as when comparing different FAPAR products.

NPL developed an approach to the problem of ensuring that adequate Quality Information is provided in Climate Data in the frame of the Copernicus Climate Change Service (C3S). The goal is to ensure that the QI associated to the relevant ECVs is sufficient for the users to make informed decision for their applications. A user survey was conducted to capture and standardize the QI of the different ECV. The scientific assessment of the different ECVs will leverage and improve upon the Fiduceo and QA4ECV projects’ outcomes. An example of the scientific assessment for FAPAR ECV is presented. As already pointed out by JRC, the main issue with FAPAR validation is the fact that in-situ measurements do not measure directly FAPAR, but this is inferred from indirect measurements. Sensor characteristics can be also very different leading to different PAR measurements. **The validation of the satellite-based retrieval is therefore challenging also considering the complexity of upscaling the in-situ measurement to the satellite pixel. In order to estimate the true value of FAPAR and establish SI traceability, a modeling approach has been used, coupled with reference traceable measurements and a full 3D characterization of the validation site.** This approach has been prototyped for the Wytham Woods forest site in UK, where a network of wireless PAR sensors, properly characterized in the lab against a reference sensor, has been deployed using a well established sampling design to allow measurement spatially comparable to satellite pixel**.** A Terrestrial Laser Scanning (TLS) system was used to reconstruct the 3D canopy structure of the validation site including realistic foliage; this is crucial in order to simulate, through a 3D ray-tracing model the "true" value of FAPAR to be compared against the in-situ measurements and to the satellite-based estimation to finally assess their quality. This approach has been defined as **"virtual traceability"** and is allows for the proper treatment of the uncertainty associated to both the in-situ and satellite measurement. The NPL site is part of the Enviro-NET network [RD-16] and collaboration with other sites that have similar 3D characterization is on going, such as the **TERN network in Australia** and the Costa Rica site.

Land Classification Algorithm (Burned Areas)

The current status of uncertainty estimation for Burned Area product in the frame of Fire CCI project was reported by UCL. This is an interesting case of allocating uncertainty information for a classification algorithm, where the output is a binary mask (burn/no burn) with estimate of day of burn. **Historically a poor or no quality information was associated to such binary flag products,** except for a quality layer providing some general hints on the confidence of the classification, such as the case for MODIS burnt area product. In the frame of the Fire CCI project, this issue is being addresses, and an effort is being put on providing probability information of a burnt pixel, instead of a simple binary flag. A dedicated framework was also developed in order to validate this probability information, using simulated burnt area maps and investigating the reliability of the probability information when adding realistic noise to the simulated data. Some questions remain on how to effectively perform full error propagation for such classification problem, in particular since the relevant algorithm are highly non-linear. The outlook of the project includes the provision of a Probability Density Function (pdf) to be associated to each pixel. **As a general recommendation for classifier algorithm is to move toward a probabilistic approach, associating a priori information to each pixel and providing as output the a-posteriori pdf,** this will help also the gridding of the output to a climate grid, which is often used for such product.

3.2.3 Level 2 Ocean Color products

As for the land products, the first step in Level 2 processing over water is the atmospheric correction for the derivation of the water-leaving surface radiance/reflectances. These products are the basis for deriving inherent optical properties and biophysical products for water applications. Example of uncertainty estimation for these products were presented and discussed.

MERIS/OLCI water-leaving reflectances

The current status of uncertainty estimation for MERIS/OLCI water leaving reflectance products was reported by ACRI. The atmospheric correction is based on the Bright Pixel atmospheric Correction (BPAC) approach, though there is not yet the provision of uncertainty per pixel**. The precision and accuracy of the water leaving reflectance are assessed through comparison with match-up in-situ measurements, such as those provided by MOBY and BOUSSOLE.** The comparison with in-situ shows a dependence on the water type (case 1 water shows better agreement) and a slight overall bias. An attempt to understand the observed bias was made by estimating the different sources of errors and considering both the satellite and in-situ reported measurement uncertainties. **The propagation of the TOA radiometric uncertainty to the Level 2 products explains only marginally the observed differences between satellite and in-situ, which seems dominated by the uncertainty in the applied system vicarious gains.** As outlook, a full error analysis should be made in order to fully understand the observed differences.

MERIS/OLCI OCR and IOPs

Application of the GUM principles to the problem of ocean colour products uncertainty estimation was presented. The approach, developed by Solvo, focused both on the Ocean Color Radiometry (OCR) and on the Inherent Optical Properties (IOP). Concerning the OCR, the GUM guidelines were followed to propagate the radiometric TOA uncertainty through the full processing chain. The different sources of errors along this chain are analysed, this include in particular: the vicarious gain adjustment, and the atmospheric correction. **The importance of the system vicarious calibration on the total error budget was specifically underlined, the uncertainty associated with the in-situ values, used for derivation of the vicarious gain, is dominated by the extrapolation of the in-depth radiometric measurements upward to the water surface. The atmospheric correction error budget is driven mostly by errors in the estimation of aerosol optical properties (AOT and phase functions).** AERONET data are essential to assess those sources of errors. Furthermore, the importance of taking care of the spectral correlation in the Level 1 radiometry for properly assessing the Level 2 uncertainty is demonstrated. Finally, an approach based on non-least square formalism is presented, allowing estimating uncertainty in the final bio-optical ocean colour products. As a final recommendation, the need for validating the uncertainty estimate was stressed.

Neural Network Uncertainty for Ocean Color products

Brockmann Consult presented an alternative approach for uncertainty estimation of water bio-optical products based on Neural Network (NN) technique. The approach has been developed for MERIS observations; all available spectral information, from visible to NIR, is exploited as input to the NN in order to span a wide range of water constituents' concentration, avoiding saturation effects that may occur in some spectral bands. The NN uses as input the MERIS measured TOA radiance with the associated angles and provides as output the bio-optical properties of interest (IOPs), such as Chlorophyll or Suspended Matter concentration. The NN algorithm accuracy is largely dependent on the NN architecture and on the used training dataset. A dedicated bio-optical model allowing simulating IOPs for different concentration mixture is used together with the MERIS-derived IOPs to train a dedicated NN, which allows for the estimation of uncertainties. A discussion was initiated on whether this approach is in-line with GUM guidelines on uncertainty estimation. **The proposed NN-based technique can be considered as part of the family of Monte-Carlo approaches for uncertainty estimation, in this sense it is an acceptable approach for uncertainty estimation, though, it will need to be validated carefully with more standard method.**

Sea Surface Temperature (SST)

Uncertainty estimation for SST is very well advanced, owing to its relevance for climate and modeling applications. Most of the work presented by Uni. Reading was performed in the frame of the **GHRSST (Group for High Resolution Sea Surface Temperature).** GHRSST was successful in the development of a harmonized format and approach for providing quality information in SST data, the so-called **Sensor Specific Error Statistic (SSES). The SEES provides the minimum requirement in terms of uncertainty information that should be provided to users, this concept has proven to be very effective in supporting the uptake of SST data from the modeling community. Uncertainty information in SSES is largely based on match-up database of drifting buoys. The inherent uncertainty in the in-situ SST estimation is specifically underlined, since the temperature measured from the buoys at a given depth can be very different from the skin temperature measured from the satellite.** The need for an independent assessment of the uncertainties is stressed, based on propagation of all error sources along the full processing chain, from Level 1 to Level 4 products. At each level, different source of errors are identified, which contribute to the overall error budget, e.g. radiometric noise, solar contamination, digitisation, sampling and regridding. **For each source of error, a full characterization should be made; following Fiduceo approach, in particular for identifying induced temporal and spatial correlation in the final uncertainties.** Retrieval sensitivity analysis is also used to investigate the impact of external data, such as pressure or TCWV, on the retrieved SST. The current error budget provided in the frame of SST CCI is still incomplete and several source of errors need to be fully characterized, such as NWP errors, undetected clouds and aerosol variability.

The final message is that an independent assessment of the error budget is required, in-situ measurements, such as those provided from drifting buoys, should be used to validate the estimated budget.

3.2.4 Level 2 Atmospheric products

Uncertainty estimation for atmospheric products had a long history, since this information has been always a strong requirement from the modeling community. The state of the art in the frame of Aerosol and atmospheric constituents was reported and discussed.

Aerosol

The status of uncertainty estimation in the frame of Aerosol CCI was reported by DLR. Uncertainty estimation is performed either using an **a-posteriori diagnostic** based on a validation dataset, such as AERONET, or via a **prognostic** approach, through formal error propagation method. **The bias or systematic component of the error budget can be assessed via the diagnostic approach, through validation data, while the random component can be predicted with the prognostic approach, e.g., using Optimal Estimation formalism. The a-posteriori and prior estimation obtained with the two approaches should be consistent; this is the process of validating the uncertainty.** A method is proposed for uncertainty validation based on comparing the probability distribution of predicted uncertainty to the a-posteriori uncertainties obtained with respect to AERONET dataset. **Pixel-level uncertainties are key for data assimilation studies and for consistent integration of measurements from different sensors.** The work is still on going in the frame of aerosol CCI to refine the uncertainty estimates and to investigate their dependency on season, land cover type, AOD, undetected clouds, directional effects and to properly propagate Level 2 uncertainty to the gridded Level 3 products. **The issue of undetected cloud was underlined, since it is not straightforward to characterize its impact on aerosol parameters retrieval, especially at the edges of a cloud.**

Atmospheric constituents (O3, CH4, CO2…)

The work coordinated by BIRA for uncertainty estimate in the frame of the GAIA-CLIM project [RD-17] was presented. **It is reminded that ground-based reference (m_1) and satellite observations (m_2) should be consistent within the associated uncertainty estimates (u_1 and u_2 respectively).** The relevant formula states that: $|m_1-m_2|<k*sqrt(u_1^2+u_2^2)$, where the factor k determines the level of inconsistency between the two measurement of the same geo-physical quantity. **However, in addition to the single uncertainty estimates (u_1 and u_2) another component plays a significant role in the error budget: the co-location mismatch. The co-location error must be both minimized (with more stringent co-location criteria) and fully characterized to quantify its impact in the overall error budget.** This is one of the goals of the GAIA-CLIM project, which aims to improve use of non-satellite measurement to calibrate and validate satellite estimate of relevant atmospheric constituents, such as T, O3, CH4, CO2, Aerosol. Within GAIA-CLIM a full metrological approach is adopted to work toward traceability of satellite and ground-based measurements. **A rigorous characterization of the multi-dimensional (spatio-temporal) smoothing and sampling effects of the atmospheric remote sensing system is required to properly characterize the co-location mismatch.** Examples of quantification of the co-location mismatch are shown using the OSSSMOSE tool developed at BIRA, in particular for the validation of the total ozone column. An operational tool was also developed in the frame of the GAIA-CLIM project, the Virtual Observatory, allowing the users to assess a massive archive of satellite and ground-based data with associated ancillary NWP data and a set of analysis tool for space/time collocation, match-up extraction, radiative transfer simulation and data visualization. A set of useful recommendations was additionally collected in the frame of the GAIA-CLIM project on how to improve uncertainty characterization of satellite-based data.

Data assimilation diagnostic

The potential role of data assimilation for diagnosis uncertainty and systematic issues in remote sensing data was illustrated by ECMWF. Data assimilation methods assume random Gaussian errors; biases are corrected before or during the data assimilation. Uncertainty in the satellite data is key requirement for including them into a data assimilation system, in particular the full error covariance matrix should be provided, including all the inter-channels correlation terms, example is shown for IASI. **The error covariance matrix can be derived either with a physically based approach, propagating all the estimated sources of errors, or with a statistically based approach, using a-posteriori statistics of the differences between observations and forecast. Data assimilation could be used as a complementary diagnosis tool for assessing uncertainties and identifying biases in satellite observations.** Overall, the need for improving error analysis is underlined in order to fully understand and correct observed biases, uncertainties should not be limited to instrument noise, but include all possible source of errors, such as radiative transfer, cloud screening, correlated terms should also be provided.

3.3 Discussion and Recommendations

A discussion was finally held around a set of seed questions, with the goal of gathering ideas for improving current status of uncertainty information for EO products.

- ***Mission Design*** – There is a clear need to convince the Space Agencies to support uncertainty budget estimation during the design phase of the mission, this includes:
  - i) the inclusion of specific requirements on the MRD/SRD for the instrument providers;
  - ii) the allocation of an appropriate budget to address al the relevant activities (e.g., pre-flight calibration, sensitivity analysis);
  - iii) the definition of a proper level of quality information to be included in the early phase of mission algorithm and products' definition;
- ***Pre-flight calibration*** – Some needs were identified as a result of the Fiduceo experience, which concern the pre-flight calibration activities, in particular:
  - i) the instrument providers to identify measurement equation and develop a traceability tree;
  - ii) the need to archive and maintain the key reference dataset from the pre-flight calibration and to make it available to users;
  - iii) the need to adopt a common and transparent methodology for pre-flight calibration for series of missions (e.g., AVHRR series) in order to minimize changes, which are then hampering consistency of derived FCDR;
  - iv) the call for an easier access to uncertainty budget associated to the instrument, this incudes as well the open-access to sensor simulators;
- ***Level 1 uncertainties*** – There is a recognized need on building upon the lessons learnt in the frame of the Fiduceo project and extend the developed methodologies for Level 1 uncertainty estimation to other family of sensors, in order to develop the relevant FCDR:
  - i) to improve characterization of geometric uncertainty, and the impact of resampling, geo-location, and viewing geometries in particular at the edge of large swath and for geostationary sensors.
  - ii) to address the practical Ground Segment issues associated to the provision of uncertainties at Level-1, in particular the increase in size of the relevant products
  - iii) the need for dedicated training and education of the users.
- ***Level 2+ uncertainties*** – The following needs were identified in order to improve Level 2 uncertainties:
  - i) to work on improved uncertainty characterization with priority to the following products: SR, LST, SWE, SM and any classification products, e.g., BA.
  - ii) to improve characterization of the error induced by undetected cloud, cloud-shadows and adjacency effects at the cloud edges.

- iii) to expand FRM concept and work toward operationalization of automatic network measurements for global process monitoring and to dedicated campaign for addressing specific regional processes;
- iv) to support the interaction between data producers and validation scientists to feedback insights into improved products;
- v) to follow rigorous error propagation from Level 2 uncertainty to higher global gridded products (Level 3 and Level 4), taking into account the effect of smoothing and interpolation within the regridding process.

- ***Uncertainty validation and inter-operability*** – The following needs were identified:
  - i) a rigorous error budget estimation (diagnostic) should be carried out prior to the measurements, the validation data should be used to validate the predicted uncertainty;
  - ii) FRM definition involves the development of more accurate RTM and the need for accurately quantifying the co-location uncertainty in order to validate the uncertainty, for this purpose appropriate tools should be developed, such as within the GAIA-CLIM project;
  - iii) additional theoretical advance is needed for addressing non-Gaussian errors and for developing multi-instrument validation, e.g., triple colocation;
  - iv) there is a need for agreeing on a common terminology and methodology in order to improve interoperability;
- ***Training and Education***– The following needs were identified:
  - i) to organize regular dedicated workshops for data producers, and users on uncertainty information;
  - ii) use case for uncertainty estimation should be well documented and provided to users;
  - iii) the concepts and methods should be promoted in international conferences;
- ***Benefits***– The potential benefits of uncertainty information in EO products were clearly stated: it represents an added value to the data by providing enhanced confidence on their quality, it is crucial to improve interoperability across different sensors. Furthermore, the uncertainty information can be retrofitted to the instrument expert team, allowing, on the long run, to further improve instrument specifications and meet the stringent climate requirements.

4 LIST OF RECOMMENDATIONS

This chapter summarizes the current status and identified needs arising from the Workshop.

Table 1 – Current status and identified needs for uncertainty information in Mission Design Phase.

Current Status	Identified Needs
The need for uncertainty information in the products is often postponed to the operational phase of a mission, with the resulting challenges in a proper characterization of the in-flight sensor performances and the practical issues of adapting products specifications.	**[REC1]** – Metrological principles should be embedded into Space Agencies practices in the early phase of the mission design by: i) including relevant requirements in MRD/SRD, ii) allocating appropriate budget to pre- and post-launch calibration activities, iii) defining product specification with a proper level of quality information **(→ *Space Agencies*)**
Pre-launch characterization activities are often reduced due to budget or time constraints, with resulting issues in fully understanding sensor behaviour while on-orbit. Pre-launch calibration database is most of the time undisclosed to users or protected by property rights with resulting difficulty in applying a full traceability tree in the Level 1 processing.	**[REC2]** – Space agency should ease traceability of calibration processing by: i) requiring instrument providers to identify measurement equation and develop traceability chain, ii) archiving, maintaining and making accessible to users the relevant pre-launch characterization database, iii) adopt common methodology for on-ground characterization for family of sensors, iv) providing free and open access to instrument simulators. **(→ *Space Agencies*)**

Table 2 – Current status and identified needs for uncertainty information in Level 1 products.

Current Status	Identified Needs
While radiometric uncertainty is well characterized following a metrological approach, theoretical advances needs to be made for fully characterizing geometric errors, and spatial correlation induced by orthorectification, interpolation and projection.	**[REC3]** – To foster the advances of theoretical approaches for fully characterizing geometric and spatially correlated errors in Level 1 products, such as those induced by orthorectification, regridding, projection. **(→ *Calibration scientists and ESA as promoter*)**
Provision of uncertainty per pixel in Level 1 products is at very early stage. While approach and tools, in particular for the radiometric uncertainty are mature enough, see example of S2 RUT, the impact of such implementation in the Ground Segment is substantial and it needs to be duly justified demonstrating benefits for users.	**[REC4]** – To demonstrate benefits and consolidate user requirements for the provision of uncertainty information at pixel-level in Level 1 products. **(→ *Science community and Space Agencies as promoters*)**
Usage of per-pixel uncertainty in Level 1 products is very limited, even in the case when this information could be retrieved from the products (see S2-RUT).	**[REC5]** – To support training and education activities within the EO remote sensing community for the correct usage of uncertainty information and to improve the available documentation. **(→ *Science community and Space Agencies as promoters*)**

Table 3 – Current status and identified needs for uncertainty information in Level 2 Land products.

Current Status	Identified Needs
An error budget for Land SR can be derived indirectly based on AERONET measurements of atmospheric state, as developed at NASA and recently adopted in the frame of ACIX exercise. On the other hand, independent measurements of SR are needed to further understand the uncertainty in SR products.	**[REC6]** – To sustain the effort in the development of a globally representative network of SR measurements for supporting the validation of satellite-derived BOA products. **(→ *Space Agencies in the frame of CEOS*)**
An accurate uncertainty estimate for satellite-derived Land ECVs, in particular FAPAR, is hindered by the fact that in-situ measurements are very often indirect and very rarely traceable to standards. A model approach allows addressing this issue by mimicking the signal that would be measured from a satellite and from ground-based observations. This approach is based on an accurate 3DRTM and a detailed characterization of the canopy 3D structure, which can be obtained from an active laser system (TLS).	**[REC7]** – To sustain the effort in the development of 3DRTM for improving validation of satellite based land ECVs and for attaining the required accuracy and traceability. **(→ *Algorithm Developers and Space Agencies as coordinators*)**
A large number of satellite-based biophysical products are currently provided, e.g. more than 30 for FAPAR. On the other hand, there is no consensus on a common definition for those products, in particular for FAPAR (e.g., white-sky, black sky, total, green). This complicates satellite products inter-comparison and quality assessment.	**[REC8]** – To work toward harmonization of satellite biophysical variables definition, in particular for FAPAR. **(→ *Algorithm Developers and Space Agencies as coordinators*)**
Associating uncertainty information to the output of a classifier algorithm (binary mask) is challenging by definition. The recent advances in this domain show that the probabilistic approach is the most promising. Within this approach a probability distribution function (pdf) is provided for each pixel. Additional theoretical work is still required and the benefit of such approach with respect to standard quality masks needs to be fully demonstrated.	**[REC9]** – To work toward advanced theoretical approaches for the provision of uncertainty information for classifier algorithms. **(→ *Algorithm Developers and Space Agencies as coordinators*)**

Table 4 – Current status and identified needs for uncertainty information in Level 2 Water products.

Current Status	Identified Needs
Error budget assessment for water leaving reflectances is largely dominated by the uncertainty in the in-situ measurements (e.g., MOBY, BOUSSOLE) used for the system vicarious calibration adjustment.	**[REC10]** – To improve characterization of system vicarious gain uncertainty, which dominates the error budget for water leaving reflectance products. **(→ *Algorithm Developers, Validation Scientists, and Space Agencies as coordinators*)**

Neural Network approaches to uncertainty estimation are a valid alternative and can be of value for further assessing the error budget estimated with conventional method. Though, additional theoretical advances are required to improve the methods.	**[REC11]** – To sustain the theoretical advances and the validation of Neural Network approaches applied to the problem of uncertainty estimation. **(→ *Algorithm Developers*)**
Uncertainty estimation for SST is very well consolidated owing to its relevance for climate studies. Recent advances were made both on understanding the uncertainty associated to in-situ validation measurements (e.g., drifting buoys) and in improving prior error budget estimate. The approach prototyped in the frame of GHRSST for SSES proven to be very effective for supporting the uptake of SST products by the modeling community.	**[REC12]** – To build upon the lesson learnt in the frame of GHRSST for the provision of uncertainty information in the products. **(→ *Algorithm Developers*)**

Table 5 – Current status and identified needs for uncertainty information in Level 2 Atmospheric products.

Current Status	Identified Needs
Characterization of uncertainty for Aerosol products is well advanced. Prior estimate based on propagation of error through the retrieval chain allows for estimating the random component, while biases are identified with ground-based independent data, such as AERONET. Remaining issues to be tackled are the effect of undetected clouds on aerosol retrieval accuracy. The same applies in general to most of the retrieved land, water and atmosphere variables.	**[REC13]** – To focus the theoretical work on the characterization of the uncertainty induced by undetected clouds in the retrieval, this applies not only to aerosol, but in general to most of the satellite-derived geo-physical products. **(→ *Science Community*)**
The mis-match collocation error, which is very often neglected in validation exercise, is a substantial component to the overall error budget. Recent advances were made for fully characterizing this error source, though additional work is required.	**[REC14]** – To focus the theoretical work on the characterization of the co-location mismatch error. **(→ *Science Community*)**
The potential interest of data assimilation as a diagnostic tool to identify biases in satellite observation was demonstrated. The feedback from the data assimilation to the Level 2 scientists should help improving algorithm and converging toward an unbiased solution.	**[REC15]** – To strengthen the link between the Level 2 algorithm providers and the data assimilation teams for improving assessment and validation of uncertainty. **(→ *Algorithm Providers and Space Agencies as coordinators)***

5 APPENDIX A: AGENDA

The Meeting agenda is reported here below.

Day 1, Tuesday 24 October 2017		
09:15 – 09:30	Welcome, Logistics and Objectives	Philippe Goryl, ESA
Theory		
09:30-10:00	Theory on Uncertainties	Nigel Fox, NPL
10:00-11:30	FCDR definition FIDUCEO example – from theory to implementation	Nigel Fox, NPL Chris Merchant, University of Reading & FIDUCEO consortium
11:30 – 12:30	Discussion	ALL
12:30 – 14:00	Lunch break	
Examples I		
14:00 – 14:30	Radiometric Uncertainties Tool for S2 - RUT	Javier Gorroño, NPL
14:30 – 15:00	MERIS and OLCI example – water leaving radiance	Ludovic Bourg, Nicolas Lamquin, ACRI
15:00 – 15:30	Ocean colour uncertainties: status and evolution	Constant Mazeran, Solvo
15:30-16:00	Coffee break	
16:00 – 16:30	Example of FAPAR in MERIS/OLCI	Nadine Gobron, JRC
16:30 – 17:00	Example of Neural Network uncertainties	Roland Doerffer, Carsten Brockmann, Brockmann Consult
17:00 – 18:00	Discussion	ALL
18:00 – 19:00	Drinks	
20:00	Non Hosted Dinner	
Day 2, Tuesday 25 October 2017		
Example II		
09:00 – 09:30	Sea Surface Temperature	Claire Bulgin, University of Reading
09:30-10:00	Land Surface Temperature	Dave Smith, STFC
10:00 – 10:30	Surface Reflectance	Eric Vermote, NASA
10:30-11:00	Coffee break	
11:00 – 11:30	Status of uncertainties in Aerosol_cci	Thomas Popp, DLR
11:30 – 12:00	Role of data assimilation diagnostics in uncertainty estimation for microwave satellite observations	Heather Lawrence, ECMWF
12:00 – 13:00	Discussion	ALL
13:00 – 14:00	Lunch break	

Validation		
14:00 – 14:30	Land Products Validation	Joanne Nightingale, NPL
14:30 -15:00	GAIA CLIM experience: The importance of in situ and matching process uncertainty estimation in the context of validating satellite data and satellite data uncertainties	Tijl Verhoelst, BIRA
15:00-15:30	Validation of uncertainties (Discussion)	ALL
15:30-15:45	Demonstration of "virtual observatory" tool	Tijl Verhoelst, BIR
15:45 – 16:00	Coffee break	
16:00– 17:00	Discussion	ALL
17:00 – 18:00	Recommendation/conclusion	ALL
18:00	End	

6 APPENDIX B: PARTICIPANTS

The list of Meeting's participants is provided in the following table.

	Name	Affiliation	Country
1.	Stefan Adriaensen	VITO	Belgium
2.	Wouter Dierckx	VITO	Belgium
3.	Jonathan Leon Tavares	VITO	Belgium
4.	Fabrizio Niro	Serco	Italy
5.	Steffen Dransfeld	ESRIN/ESA	Italy
6.	Ferran Gascon	ESA	Italy
7.	Clément Albinet	ESA	Italy
8.	Nikolina Mileva	ESA	Italy
9.	John Swinton	TVUK	UK
10.	Constant Mazeran	Solvo	France
11.	Javier Gorroño	NPL	UK
12.	Eric Vermote	NASA	USA
13.	Gabriele Brizzi	Serco	Italy
14.	Grit Kirches	Brockmann Consult	Germany
15.	Carsten Brockmann	Brockmann Consult	Germany
16.	Roland Doerffer	Brockmann Consult	Germany
17.	Pierre Guillevic	U. of Maryland	USA
18.	Sabrina Pinori	Serco	Italy
19.	Enzo Papandrea	Serco	Italy
20.	Magdalena Main-Knorn	DLR	Germany
21.	Amanda Hall	TVUK	UK
22.	Fay Done	TVUK	UK
23.	Claire Neil	Uni. Stirling	UK
24.	Raymond Soffer	NRC	Canada
25.	Sam Hunt	NPL	UK
26.	Adam Povey	Uni. Oxford	UK
27.	Alexander Gruber	TU Wien	Asutria
28.	Dave Smith	STFC RAL	UK
29.	Thomas Jackson	PML	France
30.	Tijl Verhoelst	BIRA-IASB	Belgium
31.	Nicolas Lamquin	ACRI-ST	France
32.	Ludovic Bourg	ACRI-ST	France

33.	James Brennan	UCL	UK
34.	Nigel Fox	NPL	UK
35.	Christopher Merchant	Uni. Reading	UK
36.	Nadine Gobron	JRC	Italy
37.	Claire Bulgin	Uni. Reading	UK
38.	Heather Lawrence	ECMWF	UK
39.	Nils Schön	ESA	Italy
40.	Gareth Davies	Serco	Italy
41.	Roberto Sabia	TVUK for ESA	Italy
42.	Raquel de los Reyes	DLR	Germany
43.	Andreas Baumgartner	DLR	Germany
44.	Béatrice Berthelot	Magellium	France
45.	Andreas Hueni	RSL	Switzerland
46.	Paolo Castracane	RHEA	Italy
47.	Birgit Heim	AWI, De	Germany
48.	Andrea Minchella	ADS	UK