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Applying uncertainties to ocean colour data

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Abstract
Retrieval of operational optical products from the future Global Monitoring for Environment and Security (GMES) Sentinel-3 mission aims to provide continuity of existing missions delivering ocean/land colour, surface temperature and sea surface topography data. This paper describes the current status of the Sentinel-3 Level 2 Optical Prototype Processor (O-L2PP) whose development includes not only a list of products, but also associated uncertainty estimates—a key requirement for the processor. Examples of the approaches adopted within the Ocean and Land Colour Instrument (OLCI) processing module demonstrate how uncertainties can be estimated.

(Some figures may appear in colour only in the online journal)

1. Introduction

The Sentinel-3 satellite, scheduled to launch in 2013, is the third in a series of five space missions within the European GMES programme. The programme is aimed at delivering environment and security monitoring services (covering areas such as climate change, sustainable development and environmental policies) that will be devoted to oceanography and land vegetation monitoring including fire detection and radiative power mapping. The mission aims to produce consistent long-term datasets with both an improved accuracy and reliability, and carries both an advanced radar altimeter and visible–infrared optical imaging instruments; this paper concentrates on the Ocean and Land Colour Instrument (OLCI), which is based on Envisat's Medium Resolution Imaging Spectrometer (MERIS) instrument. Applicable Sentinel-3 user requirements were identified through surveys conducted within the relevant user groups: Operational and Institutional Oceanography Groups; Oceanographic Research Users; Land Users. In the long term a series of satellites, each designed for a lifetime of 7 years, is designed to provide an operational service over 15 to 20 years.

Work is ongoing within the ESA funded Sentinel-3 project titled 'Sentinel-3 L2 product and algorithm definition' with ARGANS Ltd as the prime contractor and sub-contractors including ACRI-ST, Brockmann Consult, RAL (Rutherford Appleton Laboratory) Space and Telespazio S.p.A. alongside several European research institutions and universities (Sentinel-3 L2 Products and Algorithm Team):

- Chris Merchant, University of Edinburgh, UK
- David Antoine, Laboratoire d'Océanographie de Villefranche (LOV), UK
- Fred Prata, Nilu, Norway
- Gerald Moore, Bio-Optika, UK
- Jadunandan Dash, University of Southampton, UK
- John Remedios, University of Leicester, UK
- Jurgen Fischer, Freie Universität Berlin (FUB), Germany

- Martin Wooster, King's College London, UK
- Nadine Gobron, Joint Research Centre (JRC), Italy
- Peter North, University of Swansea (UoS), UK
- Richard Santer, LISE, Université du Littoral Côte d'Opale, France
- Roger Saunders, UK MetOffice, UK
- Roland Doerffer, Helmholtz-Zentrum Geesthacht Centre for Materials and Coastal Research (formerly GKSS Research Centre), Germany.

The overall product tree structure is based on the MERIS and Advanced Along Track Scanning Radiometer (AATSR) heritage plus the continuity of the SPOT-VGT mission (availability of the full spectral range provided by the two instruments), integrating the individual sensor (OLCI and Sea and Land Surface Temperature Radiometer, SLSTR) and synergy (SYN) processors within a single environment. This single environment is called the Sentinel-3 O-L2PP, which will be launched through the Optical Data processor of the European Space Agency (ODESA) interface that will allow the user to follow the execution either using output from Standard Output/Standard Error directed to the terminal window or through feedback displayed in a graphical user interface.

The project is organized into several distinct steps (definition, specification, implementation and maintenance) with responsibly assigned to the various partners. Phase 1 was concluded with a Preliminary Design Review (PDR) in September 2009 and the next step (the Critical Design Review, CDR, closed end 2010) has involved finalizing the Algorithm Theoretical Basis Documents (ATBDs) and hence methodologies for determining uncertainties. The list of ATBDs is extensive with 21 in total where each describes one or more algorithms, the breakup being 17 for OLCI, 3 for SLSTR and 1 for SYN processing branches.

Listed below are the OLCI processing steps/products:

- Pre-processing:
  - Pixel classification
  - Gas corrections, instrumental corrections and confidence check
  - Water vapour product
- Ocean Branch:
  - White caps and (sun) glint correction
  - Standard Atmospheric Correction (SAC) over clear and turbid (bright) waters
  - Alternative AC (AAC)—use of a Neural Net to perform the atmospheric correction including a sun glint correction
  - Ocean colour for clear and turbid waters plus transparency products
  - PAR (Photosynthetically Active Radiation)
  - ICOL (Improved Contrast between Ocean and Land processor) adjacency correction; an adopted ATBD to be implemented over a longer timescale
- Land Branch:
  - Rayleigh correction over land
  - FAPAR (Fraction of Absorbed PAR)
  - OCTI (OLCI Terrestrial Chlorophyll Index).

2. Uncertainties

For each Sentinel-3 O-L2PP product, the aim is to determine a method that will allow error estimates/uncertainties to be calculated on a pixel-by-pixel basis. However, as the science is at different levels of maturity the proposed algorithms and uncertainty estimates span an operational readiness range.

The Quality Assurance framework for Earth Observation (QA4EO), see http://qa4eo.org/, was established and endorsed by the Committee on Earth Observation Satellites (CEOS) as a direct response to a call from the Group on Earth Observations (GEO). It is suggested that data generators need to

- Assign to all data/information products a Quality Indicator (QI), which allows stakeholders to unequivocally evaluate the products' suitability for a particular application.
- Provide a definition for each QI. This should be based on a quantitative assessment of its traceability to an agreed reference or measurement standard (ideally SI), but can be presented as numeric or a text descriptor, providing the quantitative linkage is defined.

Therefore, the quantification of errors (difference between the value and best estimate of the 'true' value of the measurand) allows potential users to evaluate the products without having specialized knowledge. In addition, satellite products are increasingly assimilated into oceanographic numerical models and it is inappropriate for these users to assume the products have no error associated with them. As well as quantifying the error coming from the sensor performance (Level 1 input) plus processing, it is important we recognized that a pixel (spatial resolution from hundreds of metres to approximately 1 km) will have spatial variabilities within it. Therefore, when comparing satellite with *in situ* bio-geophysical products, uncertainties (dispersion of the quantity values) will contain a mixture of this sub-pixel scale variability and satellite product quantifiable error. Also, including pixel-by-pixel uncertainties has the potential to double the size of the products. However, it is foreseen that the implementation of NetCDF v4 with data compression will be used to partly offset this growth in product size and network speeds will continue to improve with external impetus imposed by the general public increasingly using the internet to download high volume content such as videos and films.

The two OLCI examples provide examples of uncertainties that have been calculated at a stage when the instruments are still being built and so only simulated data are available.

2.1. Example: sun glint

The OLCI sun glint correction ATBD (Lavender and Kay, 2010, OLCI Glint Correction ATBD SD-03-C09 v2.0) was developed from the heritage of the MERIS (Montagner *et al* 2003) and Sea-viewing Wide Field-of-view Spectrometer, SeaWiFS (Wang and Bailey 2001) approaches; sun glint refers to optical radiation reflected from the ocean towards the sensor in a near specular manner. The amount of sun glint will be reduced compared with MERIS as the OLCI field-of-view (FOV) is tilted to reduce the sun glint pollution (maximum operating zenith angle of 55°).

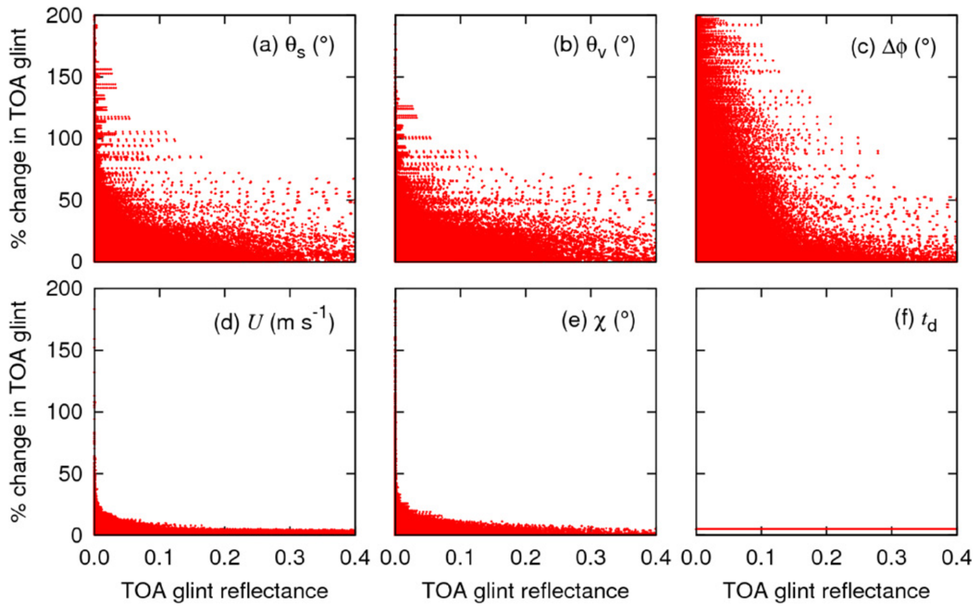

Figure 1. Percentage change in Top Of Atmosphere sun glint reflectance for 5% change in six input variables (solar zenith angles, viewing zenith angle, solar viewing azimuth, wind speed, wind direction and diffuse transmission from (a) to (f)) against Top Of Atmosphere sun glint reflectance.

For MERIS, all water pixels are tested for sun glint by comparing the reflectance with the predicted sun glint reflectance, ρ_g (Montagner *et al* 2003):

$$\rho_g = \frac{\pi r(\omega) p(\xi, \eta)}{4 \cos \theta_s \cos \theta_v \cos^4 \beta} \qquad (1)$$

where $r(\omega)$ is the Fresnel reflectance (approximated as a constant, 0.02, for incidence angles between 0° and 50°), $p(\xi, \eta)$ is the probability distribution function (PDF) for the sea surface slope, θ_s is the solar viewing angle, θ_v is the viewing zenith angle and β is the zenith angle of the wave facet calculated from the specular reflection angle (ω).

As the input variable (Level 1) PDFs are not currently available, current research has focused on the sensitivity analysis approach. The predicted sun glint radiance is non-linear in all input variables except the atmospheric transmittance, which itself is a function of the illumination and viewing geometries. Therefore, the calculated Top Of Atmosphere (TOA) sun glint radiance is highly sensitive to changes in the input variables in at least parts of their ranges (figure 1). This can be demonstrated by evaluating how the sun glint function changes as a result of a 5% change in each input variable, using values from across the full range of all variables (Saltelli *et al* 2006).

Figure 2 and table 1 show an example of sensitivity estimation for six pixels in a MERIS image. In this case, the wind speed has been varied by 5% and the corresponding change in sun glint reflectance is shown. The uncertainties in the low sun glint region will not impact on the final uncertainty as these reflectances are too low to be considered as medium sun glint. However, the uncertainty at pixel C will lead to uncertainty in the corrected reflectance and the uncertainty at D could change the classification of the pixel as high/medium sun glint.

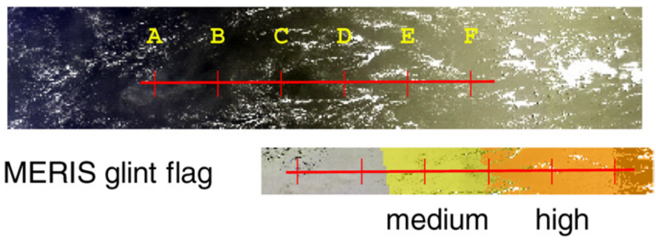

Figure 2. Section of a MERIS image of the Pacific Ocean, showing the position of six pixels (A–F). Main view is a Level 1 RGB image with the pixel also shown in reference to the application of the sun glint flag.

Table 1. Sun glint reflectance and uncertainty produced by a 5% change in wind speed for the six pixels shown in figure 2. Atmospheric transmittance has been taken as 1.

Position	Sun glint flag	TOA sun glint reflectance	Absolute uncertainty	100 × Relative uncertainty
A	None	0.0008	0.0001	14.8
B	None	0.0027	0.0003	9.6
C	Medium	0.0125	0.0008	6.1
D	High	0.0233	0.0010	4.5
E	High	0.0492	0.0011	2.2
F	High	0.0834	0.0003	0.3

This illustrates how uncertainty in the calculated sun glint radiance can lead to two types of error:

- Uncertainty in the size of the corrected radiance for the medium sun glint region (e.g. pixel C in figure 2). This will lead to an uncertainly that propagates along the downstream processing chain.
- A pixel can be wrongly categorized as low, medium or high sun glint (e.g. pixel D in figure 2). This is more

difficult to quantify at later stages of processing, but can at least be reported to the user.

It remains to be determined how many repeated runs are needed to give an accurate estimate of uncertainty. For the six pixels used here, 100 runs gave a relative uncertainty consistent to within 3% to 4%, and a mean sun glint within about 3% of the reported value while 1000 runs gave consistency in the uncertainty to 1% to 2% and a mean within 1% of the reported value. Increasing further to 10 000 runs gave more reliable results, but may be very demanding in terms of computation time for practical use if this approach is to be run in real time.

2.2. Example: atmospheric correction

In order to determine the errors resulting from the OLCI SAC, combination of a clear water atmospheric correction and bright water adjustment, a sensitivity analysis has been performed by ACRI-ST (Lamquin 2010—Error Propagation in the Atmosphere Correction Technical Note v1.2). The two near infrared wavelengths used for the determination of aerosol properties in the AC algorithm of MEGS (MERIS prototype processor) have been modified with additive Gaussian noise. Then, statistics of departures from the original retrieval (selection of aerosol models, marine reflectances, etc) have been computed for MERIS observations.

As computation of output uncertainties from noise simulation is very time consuming in near-real time, the aim is to create look-up tables; these will be built once and then called during data retrieval for faster error estimation. A preferred method is based on an equation linking the water-leaving reflectance to the atmospheric path (Rayleigh+aerosol) reflectances and transmission as it directly relates the error in the near infrared to output reflectances at other wavelengths. The tabulation of the relationships between these quantities and the aerosol optical depth has been tested and showed that water-leaving reflectance (ρ_{surf}) can accurately be determined by a comparison between computed and simulated uncertainties for a single bracketing pair of aerosol models (see figure 3).

3. Discussion and conclusions

The Sentinel-3 Prototype Optical Processor has progressed from specification to implementation, but this paper primarily deals with the approach adopted for providing pixel-by-pixel based uncertainty estimates within the OLCI processor. Determination of Quality Indicators is not easy, but is seen as a real benefit to the eventual users of the data. There is an assumption that Level 1 will derive uncertainties so that these can feed into Level 2, but uncertainties will also be needed for auxiliary data and the algorithm/modelling process (at each step/known assumption).

The sun glint example showed the highest sensitivity to the input values (figure 1) at low sun glint values and the consistency (table 1) was also much worse for the low sun glint values, but this should not matter as the values are below

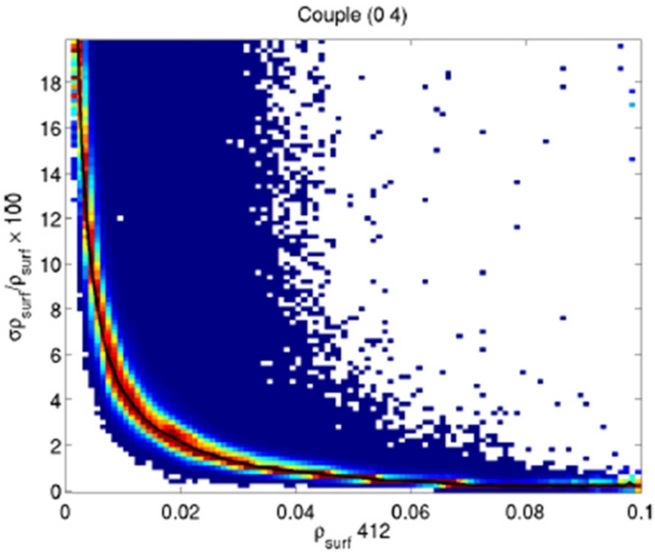

Figure 3. Histogram of uncertainty in surface reflectance versus surface reflectance with its corresponding median curve (fitting the histogram maximum value), at 412 nm, for a specific geometry and bracketing pair of aerosol models (0, 4). Source: Lamquin (2010) Error Propagation in the Atmosphere Correction Technical Note v1.2.

the medium sun glint threshold and so do not undergo a sun glint correction. Also, the use of 5% is an arbitrary decision and may not reflect the true variation in each input variable. The atmospheric correction example was similar to that used for sun glint—multiple runs with additive Gaussian noise. As noted, the computation of output uncertainties from noise simulation is very time consuming in near-real time and so therefore the approach taken is to fit a median curve to the data (figure 3). The median can be fitted so that the curve's coefficients can be stored in look-up tables.

Acknowledgments

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