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Contract Report to the European Space Agency

Milestone 1 Tech Note - Part 2: IFS Interface

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Milestone 1 Tech Note - Part 2
ESA/ESRIN Contract 20244/07/I-LG

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Abstract

Contracted by the European Space Agency (ESA), the European Centre for Medium-Range Weather Forecasts (ECMWF) is involved in global monitoring and data assimilation of the Soil Moisture and Ocean Salinity (SMOS) mission data. To this end ECMWF has developed the Community Microwave Emission Model as the passive microwave forward model operator to simulate brightness temperatures (TB). ECMWF has also developed a series of fortran routines and shell scripts which makes it possible to interface SMOS data in the Integrated Forecast System (IFS) of ECMWF. The technical implementation of the IFS interface will permit the monitoring of SMOS TB over land and sea. This report is the Part 2 of the first Milestone Technical Note / Progress Report of the ESA Request for Quotation RfQ 3-11640/06/I-LG. It provides technical documentation of the IFS interface with SMOS data.

1 Introduction

With the launch of the Soil Moisture and Ocean Salinity (SMOS) satellite, an unprecedented new source of remote sensed data sensitive to soil moisture will be made available for scientific purposes. The European Centre for Medium-Range Weather Forecasts (ECMWF) will have access to a near real time (NRT) product (level-1C brightness temperatures), automatically downloaded via ftp from the Data Processing Ground Segment (DPGS) server. To take fully advantage of this NRT product, ECMWF is currently carrying out the technical implementation of this new data type in the Integrated Forecast System (IFS). The ultimate goal of this phase is the operational monitoring of brightness temperatures (TB) over land and sea. This, among others, will make it possible to report preliminary strengths and weaknesses on first SMOS data and contribute at key decision points during the commissioning phase. The main steps involved in this phase are the following:

a.- Conversion of NRT Binary Universal Form for the Representation of meteorological data (BUFR) product to internal ECMWF BUFR format.

b.- Pre-screening of BUFR data (thinning and consistency checks).

c.- Conversion of SMOS BUFR data to internal Observational Data Base (ODB) format for use in the IFS.

d.- Computations in model space of observations with model fields.

In order to technically implement all these steps, a few simulated SMOS files from the Level-1C NRT processor were available. These files were simulated for the future months of Dec. 2010 and Nov. 2012. ”Future” data is not accepted in the IFS, since among others, background atmospheric fields are not available for future dates. Thus, several adjustments in ECMWF scripts have been necessary in order to make these test files compatible with present experiments.
This report provides technical documentation on the IFS interface with SMOS data. It is produced as Part 2 of the first Milestone Technical Note / Progress Report [MS1TN-P2] and it is complementary to the MS1TN-P1 which describes the global emissivity model CMEM.

2 Conversion of NRT BUFR product to internal ECMWF BUFR format

SMOS NRT products will be processed at the European Space Astronomy Centre (ESAC) in Madrid (Spain) and sent to ECMWF via the DPGS interface. Before being used by ECMWF BUFR software, BUFR data received by the NRT processor will go through a straightforward process, which consists in transforming the

BUFR NRT product into a version compatible with ECMWF software. This process will be done automatically by the operations department. As input, files with the format ”*miras_YYYYMMDD_HHMMSS_ YYYYMMDD_HHMMSS_smos_$orbit_o_YYYYMMDD_HHMMSS_l1c.bufr*” as defined in the file name convention of the SMOS NRT BUFR specification document, will be received at ECMWF. The output of this process will be files with the format *SMOS0001YYYYMMDDHH.DAT*, representing 6 hours worth of data. These pre-processed files are stored in ECMWF archive systems MARS (Meteorological Archival and Retrieval System) and ECFS (ECMWF File Storage system). MARS is the main repository of meteorological data at ECMWF. It contains terabytes of operational and research data as well as data from special projects. SMOS data will be stored in the MARS archive for research assimilation experiments. ECFS is the Centre’s archive/retrieval system for user files. It runs on a series of dedicated IBM machines, and can be accessed from all major platforms by Unix like commands. For passive monitoring of SMOS data, pre-processed files will be fetched from ECFS (available in the path ec:/emos/e/SMOS/), ready to be used for consistency checks. More details about this operational chain of format conversion will be given in the second Milestone Technical Note / Progress Report [MS2TN-P2] at T0+8.

3 Pre-screening of BUFR data

Before SMOS observations are loaded into the Observational Data Base (ODB) as input for the IFS, the data undergoes a pre-screening process. Pre-processing of SMOS BUFR data involves several steps:

1. Files which fail to contain crucial header information are rejected: it is checked that files are encoded in BUFR format, date and time are complete, geographic coordinates are not missing and instrument data corresponds to SMOS data,
2. Validity of data is checked:
    - Individual observations are checked to be in a correct geographical position,
    - TB are checked to be in the range of physically reasonable values (not lower than 50 K and not greater than 350 K),
3. Data is thinned to reduce data volume of SMOS files as input for the IFS.

This series of jobs has been implemented within the Supervisor Monitor Scheduler (SMS) analysis family, under the name *presmos* in the *prepare_obs* subfamily, as shown in Fig. 1. Data thinning is a critical step in the way that it selects which data from the original BUFR files will be monitored by the IFS scripts. Thinning can be done in many different ways. Several experiments have been carried out in order to investigate the optimal way of reducing the very large SMOS files.

Data thinning

The SMOS observing system senses a single surface pixel with many different incident angles. The angular resolution is very high, and thus pre-processed observation files contain lots of information. Hence, SMOS BUFR files can be very large, close to 1 Gbyte of data volume per time-slots of 6 hours worth of satellite data. This amount of data cannot be handled in the IFS just for a single satellite instrument, taking into account that many other satellite data are used simultaneously. Thinning is therefore necessary. In order to investigate the optimal thinning of SMOS BUFR files, several experiments have been carried out. In the first experiment (EXP1), only subsets of BUFR messages containing incident angles multiples of 1 degree ($\pm$ 0.01) are selected

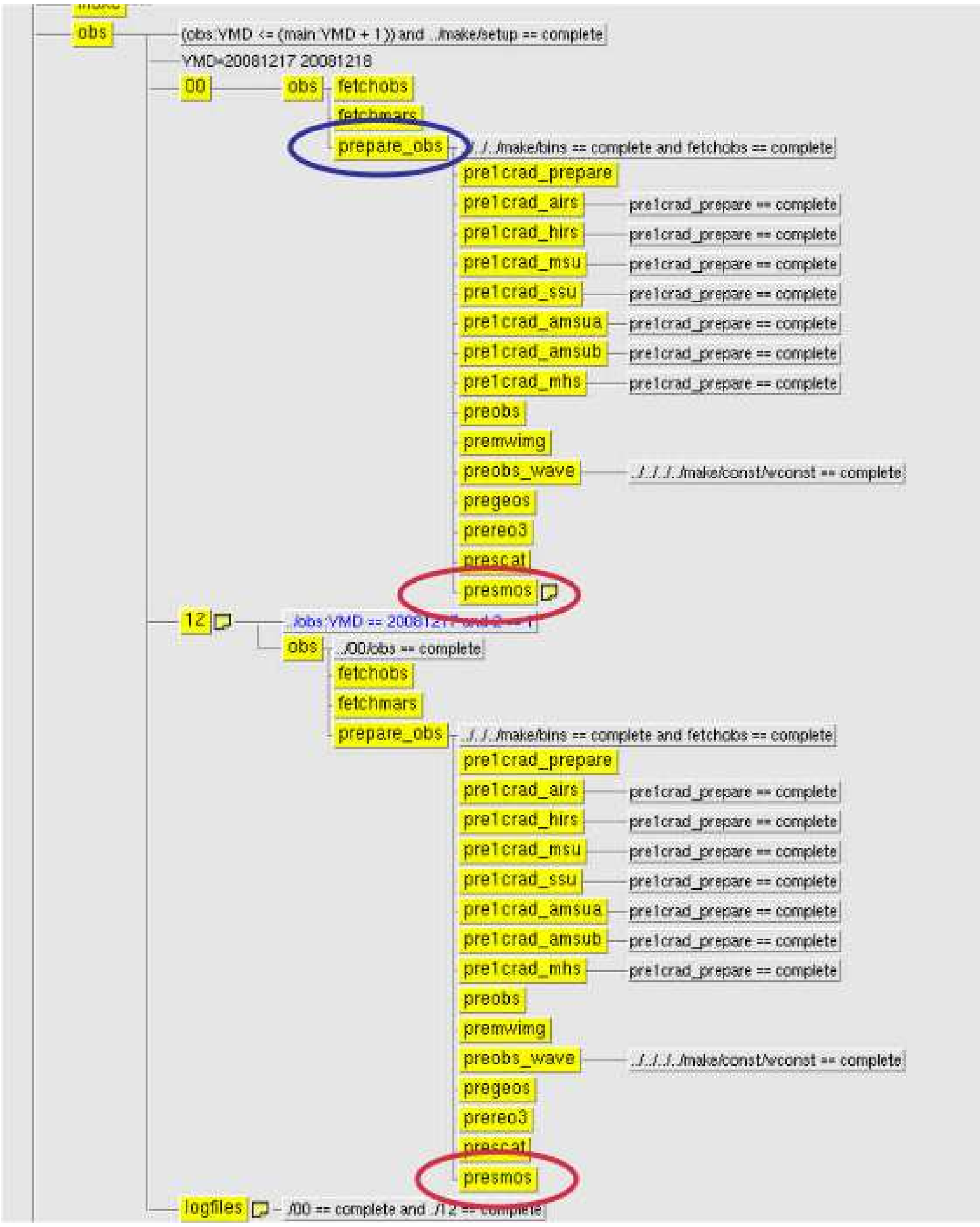


Figure 1: Presmos jobs within the analysis family of the SMS.

and pass the filter. The rationale for this is that, even though land emission is not a linear process with the incident angle, the microwave emission should not change very much for a difference of 1 degree in the incident angle. Moreover, field experiments which have investigated the land emission at L-band used only a few number of incident angles, generally multiples of 10, and thus there is not much known about which angular resolution is needed to effectively observe a difference in microwave land emission. In the second experiment (EXP2), a simple filter which keeps only one out of 10 subsets of a BUFR message has been applied. This filter roughly corresponds to a data reduction of 90% of the original file. The test file used for these two experiments corresponds to a SMOS-simulated file by the Level-1C TB processor for the 17^{th} of December 2010. The first 6 hours of data of this file after thinning with EXP2 are shown in Fig. 2.

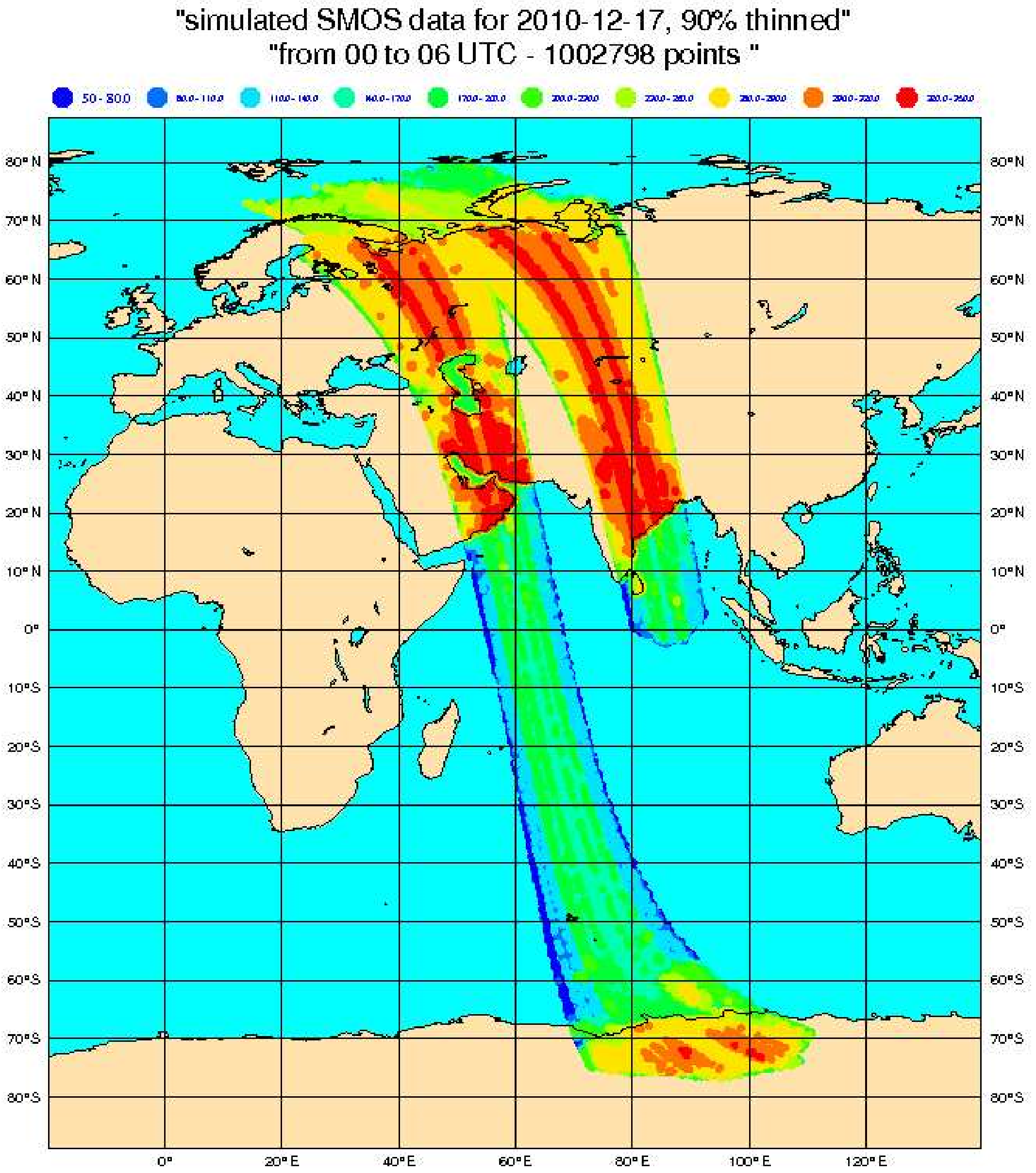


Figure 2: Simulated SMOS observations thinned by ∼ 90% from 00-06 UTC on the 17^{th} *Dec. 2010. (EXP2)*

For testing purposes, the original BUFR testing file in these two experiments has been split into 20 parts, and just one of them is shown here. The split file contains several snapshots covering mostly ocean, whereas it also observes some land. The satellite track which corresponds to this file is shown in Fig. 3. In total, it has a volume of 1067724 bytes, corresponding to 48993 observations. The histogram of simulated TB is shown in Fig. 4a. The mean is 108 K whereas the standard deviation is 39.1 K. Fig. 4b shows the histogram of TB for EXP1, i.e., when only subsets of BUFR messages which contain incident angles multiples of 1 degree ($\pm$ 0.01) are kept. In this case, only 67 observations passed the filter from the original 48993 observations, and thus a) an insufficient number of observations will be loaded in ODB for monitoring purposes and b) statistics change dramatically. In Fig. 4c, the histogram of TB which corresponds to EXP2 is shown. As observed, the number of remaining observations is approximately 10% of the initial number of observations, and the statistics are very similar, while also keeping a large number of incident angles. Applying a simple filter like this reduces the data

volume by $\sim$ 90%, but a significant number of observations will still be loaded into ODB and monitored.
For EXP1, it could be argued that a different data selector (for instance, choose integer incident angles $\pm$ 0.1 degrees) could increase the number of observations that pass the filter. However, it is difficult to optimize the angular filter criteria to control the number of selected observations and furthermore it would depend on the geographical position of the observations. In any case not all angles could be monitored in a second phase. Thus, using a filter-type as in EXP2 is preferred to a criteria based on incident angle values. All these experiments have to be checked with real SMOS data for which the incident angle effect might be different compared to simulated test data.

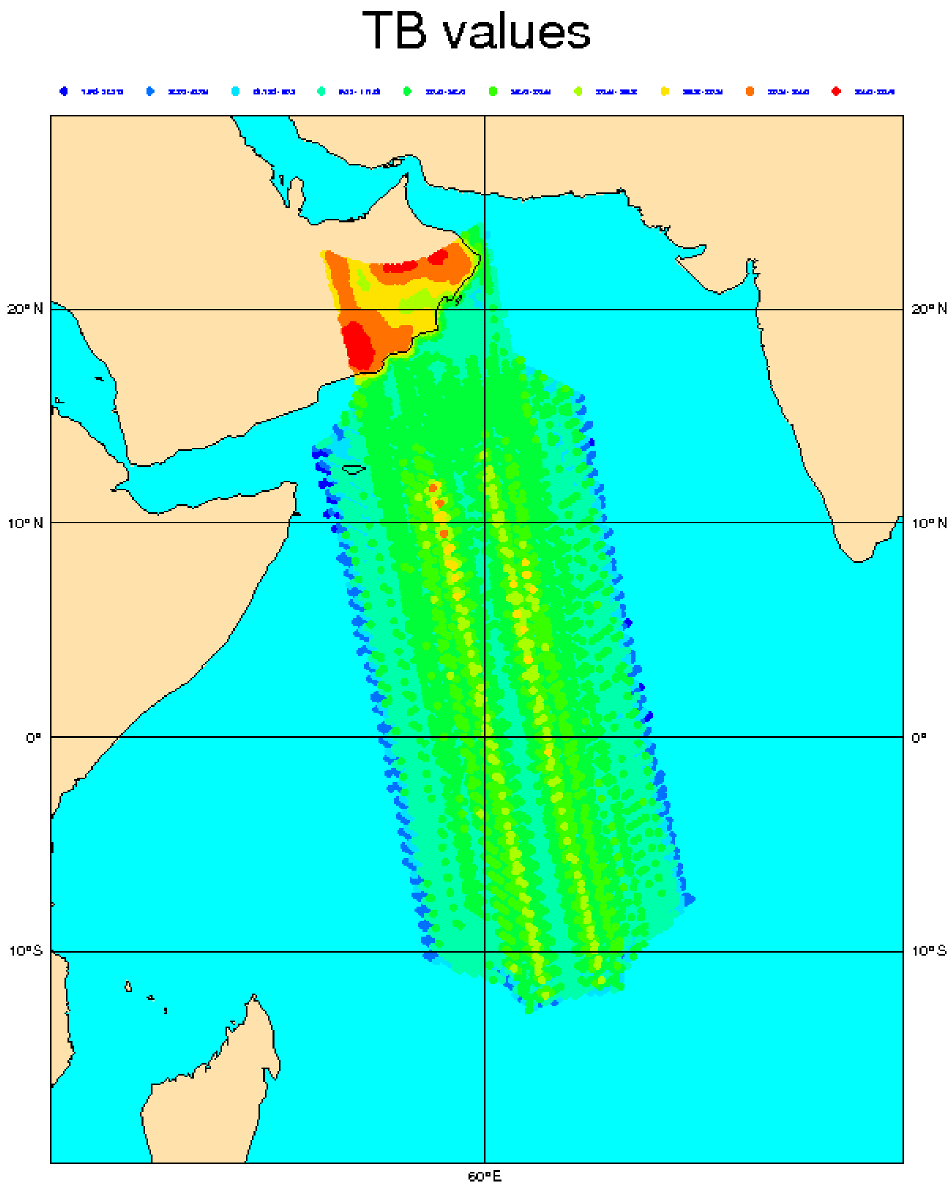
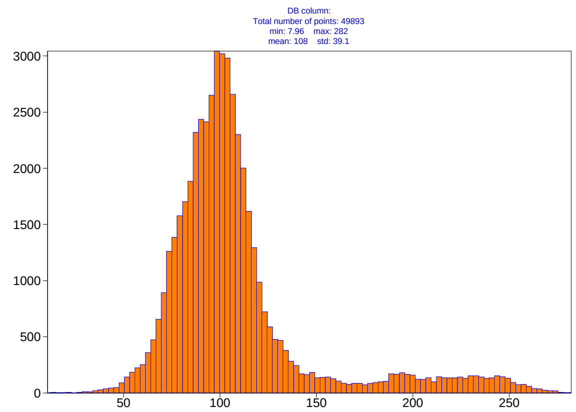


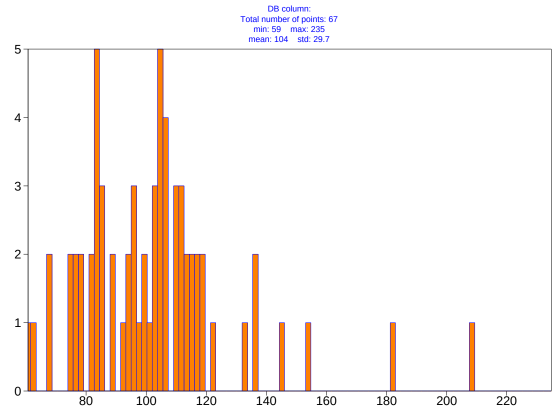
Figure 3: File used (reduced from original file) for pre-screening jobs in EXP1 and EXP2.

Even though SMOS BUFR messages also contain information about the quality of the observations, at this

(a) Histogram of TB for testing file



(b) Histogram of TB for EXP1



(c) Histogram of TB for EXP2

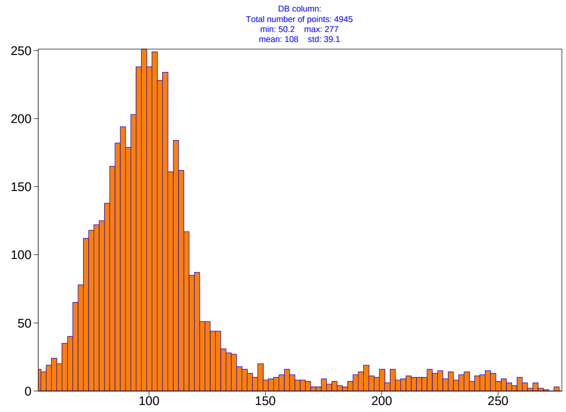


Figure 4: Histograms of TB.

stage we prefer not to reject data based on observation quality flags. In this way, geographical areas, time periods or data with specific incident angles, where the data may have a problem can easily be found during the monitoring step. And this is because during the monitoring step data can be discriminated as a function of observational flags and plotted, for instance, as time-average geographical mean fields. Otherwise, an overall quality assessment of the SMOS observations as a function of geographical location, time or incident angle would be more difficult to be produce.

4 Mapping BUFR messages to ODB

At the end of the pre-screening step, the reduced, consistent set of SMOS data observations are re-encoded in BUFR and then supplied to the ODB loader. The Observational Data Base (ODB) can store and retrieve large amounts of meteorological numerical data in an efficient manner while used from within the IFS model. ODB software mimics relational database queries through its ODB/SQL -compiler and data can currently be accessed through ODB-tools in READONLY mode or via a Fortran90 interface layer. The conversion to ODB is possible by assigning SMOS BUFR messages type and subtype codes and SMOS observations type and subtype codes, as well as the definition of several variables which project the information from BUFR to ODB systems:

SMOS BUFR		SMOS ODB
type code (30)	$\mapsto$	observation type (SATEM [7])
subtype code (203)	$\mapsto$	subtype code (400)

Further, a new ”smos” table has been created, which stores all the information contained in each BUFR message as input for retrieval in the IFS.

5 Computations in model space

SMOS TB will be monitored for a specific number of incident angles and for H-V polarisation. For these angles, TB will be monitored at global scale, as well as departures from the background values simulated with the CMEM forward operator (see Milestone 1 Tech Note, Part 1).
There are basically two options to compute SMOS first-guess departures: in observation space or in model space. In the case of SMOS, first-guess departures will be computed in model grid points following the approach of [2]. Either in observation or model space, surface heterogeneities need to be accounted for soil moisture retrieval. In the IFS, the implementation of the microwave forward model operator and computation of first-guess departures in model space adds several advantages: 1/ it allows to take advantage of the already existent structure for the implementation of all-sky observed radiances of AMSRE and SSMI data, including the optimal parallel computation on ECMWF supercomputers; 2/ all the background fields necessary to simulate TB at the top of the atmosphere are available in model grid points through the model physics (callpar routine). Thus, avoids to interpolate physical quantities to observation location; 3/ AMSRE radiances in C-band will also be assimilated in research experiments to retrieve soil moisture, and SSMI will be effective when little knowledge about surface emissivity is given. First-guess values for both types of data is currently computed in model space.

Fig 5 shows a general organigram about how Level-1C SMOS data received at ECMWF is interfaced in the IFS. Observations which survive the pre-processing jobs are mapped into ODB and further they go (roughly) through a three-steps phase:

1. Observations are brought to model grid-point space using the nearest neighbour technique,
2. Observations are compared to background TB simulated with the forward model operator in grid-points,
3. Observations and background TB are feed back to observation space, and stored in ODB tables.

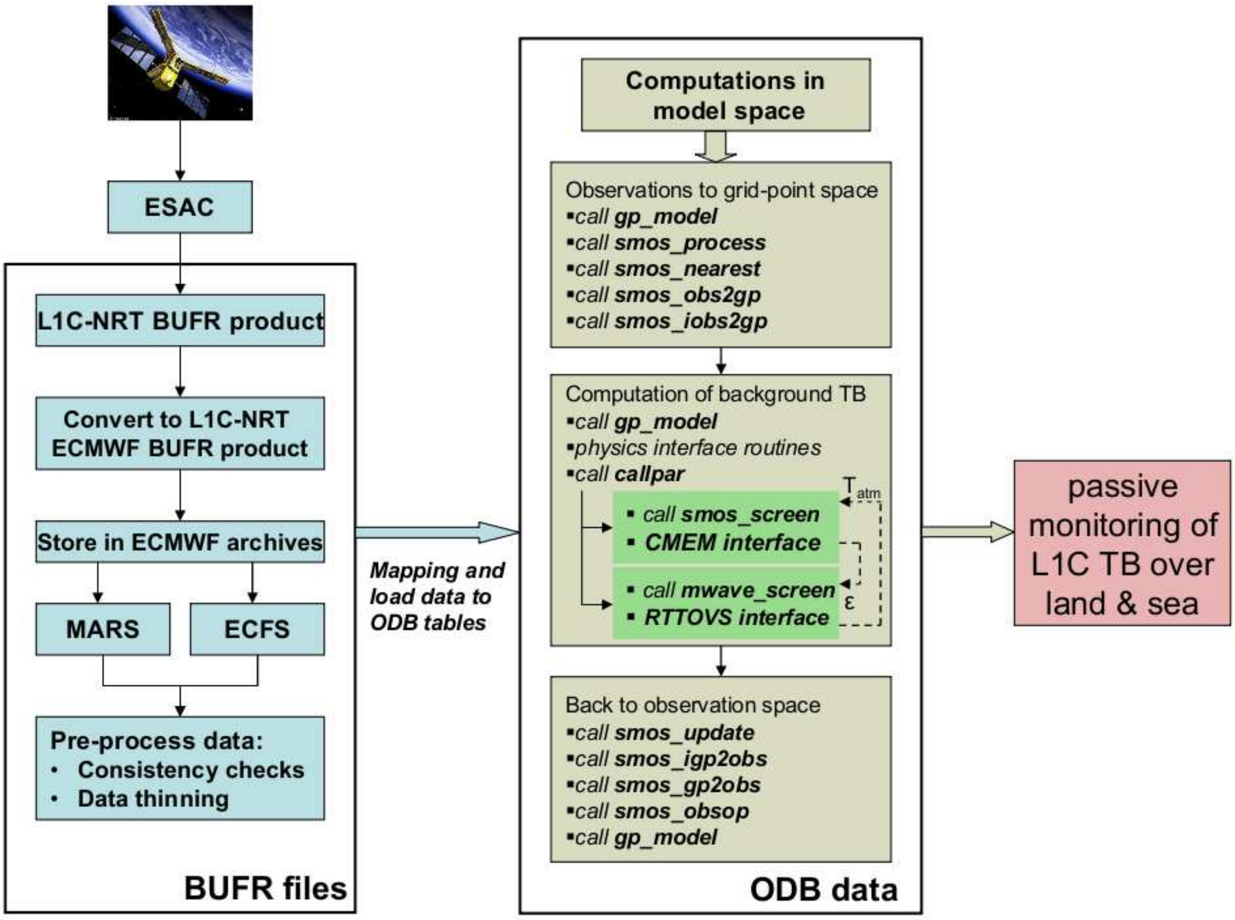


Figure 5: IFS interface organigram and general path that SMOS observations will follow before operational monitoring products will be obtained.

All these three steps are accomplished through the call to several routines which have been implemented in the IFS (see the ODB data box in Fig. 5). These routines will be part of the next cycle CY36R3. The main purpose of the routines which bring observations to grid-point space is:

gp_model: prepare computations in grid-point space at the required resolution;
smos_process: get SMOS observations from ODB to grid-point space;
smos_nearest: find nearest grid-point to each SMOS observation;
smos_obs2gp: get SMOS observations from observation space to grid-point space using parallel computation;
smos_iobs2gp: get SMOS mask (flags) from observation space to grid-point space using parallel computations ;

Fig. 6 shows SMOS observations in model grid-point for the simulated file on the 17^{th} of December 2010, after thinning 90% of all the initial observations (EXP1). Grid points correspond to a grid of resolution T159 ($\sim$ 125 Km). In Fig. 7 a zoom in over the South-Indian coast is carried out. For clarity in the plot, the T159 grid points are shown (black squares) overlapped to the nearest SMOS observations to grid points (blue circles) with the distance between grid point and observation pixel center in metres. The distance limit beyond which observations are rejected has been fixed to 10000 m. The number of observations which will be monitored depends on the model grid resolution. At T799 ($\sim$ 25 Km) for all grid points SMOS observations within the distance limit are found. Many other details will be given in the deliverable MS2TN-P1 (collocation software development) at T0+6.

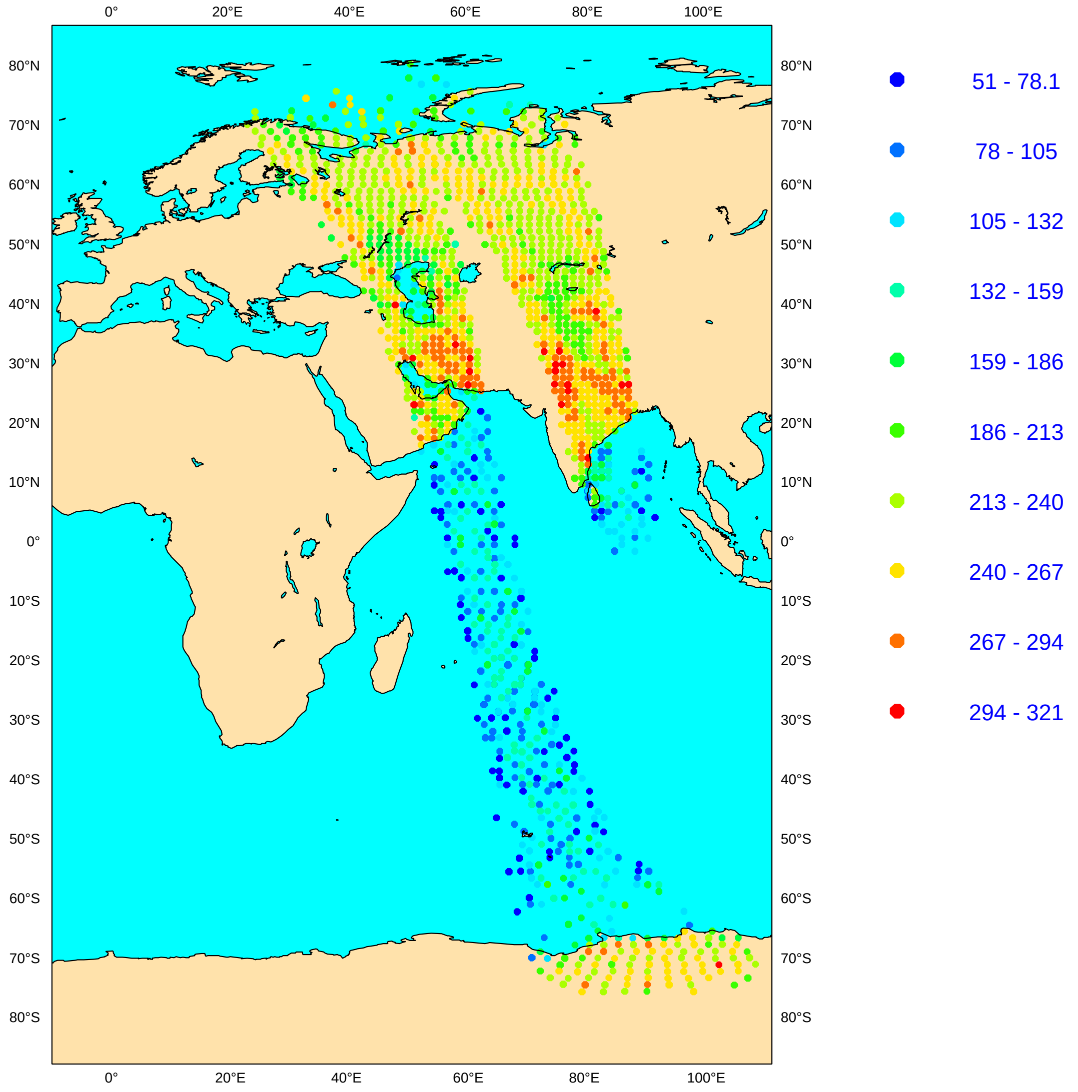


Figure 6: Collocated SMOS TB to grid-points in a T159 model grid. Values are in K.

Forward computation is conducted on model grid-point space. The Fortran 90 routines in the ”computation of background TB” box of Fig. 5 have been implemented to this end. Their main purpose is:

gp_model: prepare computations in grid-point space at the required resolution;
callpar: store all the background fields needed to run the forward model operator;
smos_screen: double check SMOS observations and select active profiles;

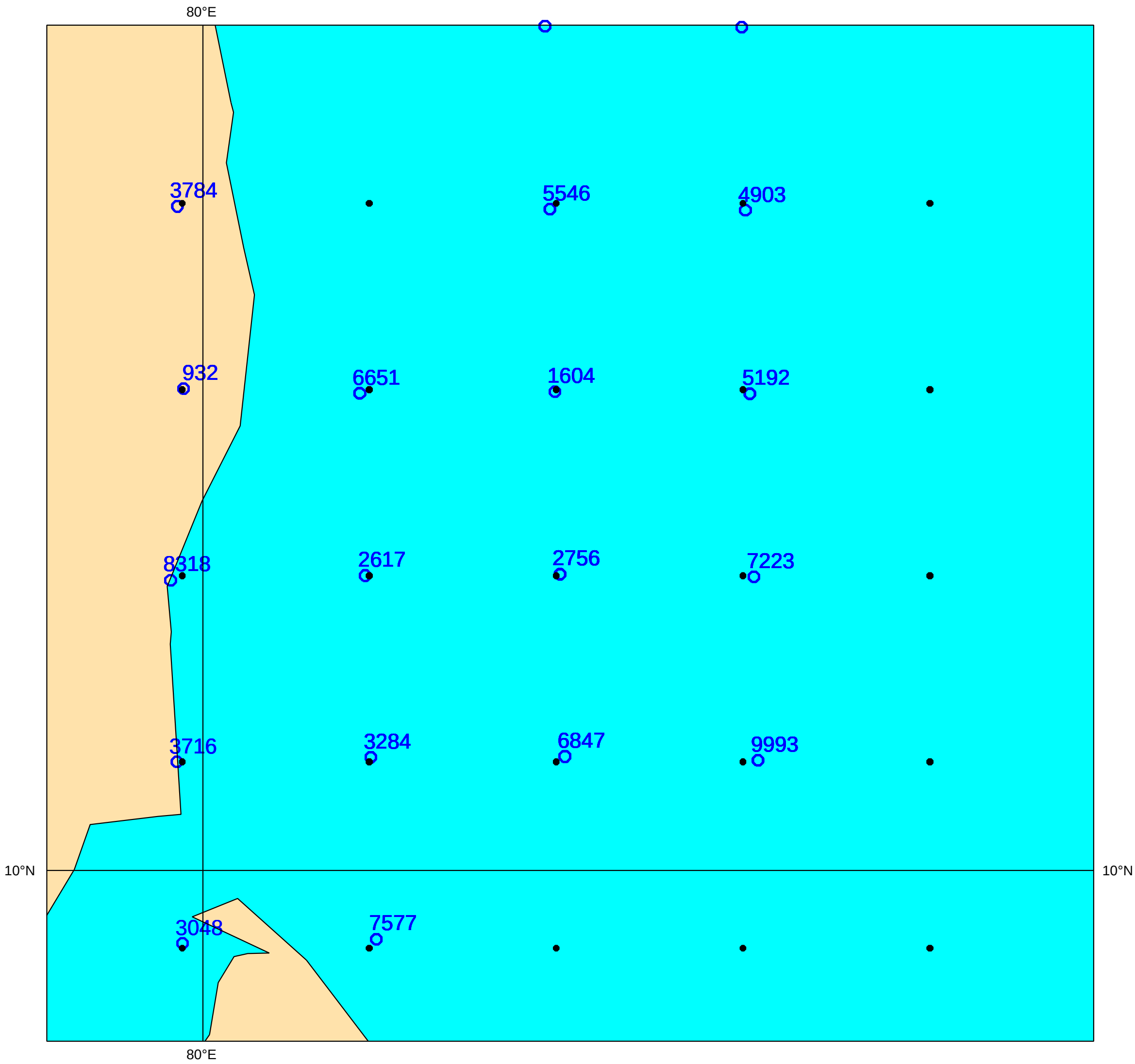


Figure 7: Nearest SMOS observations (blue circles) to grid points (black squares) in a grid of T159 spectral resolution. Values in the figure represent the distance between the model grid point and the nearest SMOS observation point, in meters.

mwave_screen: check all sky-radiances observations and select active profiles;

The RTTOVS-CMEM interface is implemented at this level (see Fig. 5). The RTTOVS (Radiative Transfer for the advanced TIROS Operational Vertical Sounder) version used is version 9, which is the last release [1]. Both packages can exchange information through several calls to the ECMWF physics package (callpar routine). RTTOVS provides the atmospheric contribution to the total TB at the top of the atmosphere for frequencies larger than 10 GHz. In turn, CMEM provides the surface emissivity to RTTOVS, thus a more realistic emissivity for the lowest atmospheric level.

Finally, before global maps of background departures or TB values are produced, observations and background values are transformed back into observation space and stored in ODB tables. To this end, the Fortran 90 routines in the "back to observation space" box of Fig. 5 have been implemented. Their main purpose is:

smos_update: Put computed brightness temperatures from grid-point space to ODB;
smos_igp2obs: Send SMOS mask (flags) from grid-point space to observation space using several processors;
smos_gp2obs: Send SMOS observations from grid-point space to observation space using several processors;
gp_model: Gather all the information and close computations in grid-point space.

As output of this process, operational monitoring products will be obtained, which will make it possible to assess the global quality of SMOS observations during the commissioning phase. This will be widely discussed in MR1/2/3 as a part of the WP1700 (T0+11, T0+14 and T0+17).

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