Open Forecast Use Cases – Definition and Requirements

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Executive Summary

This document describes the first steps to setup the use cases of the OPEN FORECAST project. It reports on the detailed definition of the two use cases, Particulate Matter Forecast Service (PMFS) and Satellite Data Service for Agriculture (AgriCOpen), and summarizes the use case requirements. For the first use case, the Particulate Matter Forecast Service, we give an introduction to the model to be used as well as the modes and additional modules which are planned to be used for the service operation. For the second use case, the Satellite Data Service for Agriculture, the different data products to become available are defined and the workflow to obtain these data products from the input satellite data is shown. In addition, the tools to obtain the different products are defined.

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2 Introduction

At the beginning of the report, we give a quick introduction into the project and the main project goals. In addition, we introduce this reports purpose.

2.1 Project Overview

The overall goal of the proposed action OPEN FORECAST is to deliver a novel Generic Service to complement the Public Open Data Digital Service Infrastructure. This HPC Open Data Forecast Service combines highly-valuable, public and open datasets with supercomputing resources to produce novel relevant data products for European citizens, public authorities, economic actors, and decision makers. Analysing datasets from two innovative application areas, pollution data and agricultural data, OPEN FORECAST provides forecast services for smart farming and smart cities. Supercomputing resources are used to compute domain specific methods on large datasets to generate forecasts on urban pollution and for precision farming. The resulting data products are public and open and will be made available through the European Data Portal. Additional publication channels include domain related data portals and APIs for the integration into stakeholder services. Furthermore, data visualization offered by OPEN FORECAST allow researchers and experts to conduct visual analyses of the data products and serve as visual communication assets towards citizens and decision makers. The whole service pipeline is "designed to be extended and to be re-used". This approach enables other European stakeholders and use case owners from other application domains to adapt their business models to the HPC Open Data Forecast Service pipeline. OPEN FORECAST exploits, wherever possible, results from European activities. This includes the usage of the eID CEF[1] Building Block and the publication of project results through INSPIRE[2] services. The data products are enriched with metadata, compliant with standards used for the European Data Portal, and APIs are provided for seamless harvesting.

2.2 Project Goals

The overall goal of the action is to combine public and open datasets with supercomputing resources to produce novel data products for European citizens, public authorities, economic actors, and decision makers. Specifically, the Action will deliver a service (the "Open Forecast service") that will take data from different sources, process it using supercomputing resources to generate open and public data products compliant with the European Data Portal.

The function of the service, which will be designed as generic as possible to potentially serve a multitude of use cases, will be exemplified through the implementation of two use cases: Particulate Matter Forecast Service (PMFS) and Satellite Data Service for Agriculture (AgriCOpen). PMFS's goal is to provide a detailed forecast for the concentration of particulate matter in the Stuttgart metropolitan area. The use case will use open sensor data from the

[1] https://ec.europa.eu/cefdigital/wiki/display/CEFDIGITAL/eID
[2] https://inspire.ec.europa.eu

luftdaten.info[3] network and public data from LGL, which will be processed with supercomputing resources. The resulting open data products will be particulate matter forecasts. AgriCOpen's aim is to provide services and products for agricultural smart farming practices based on open satellite imagery data like Sentinel-2[4]. It will use public open spatial data from the Sentinel-2 satellite mission. Data will be processed via supercomputing resources.

The resulting open data products will be agricultural forecast data (crop parameters, yields, productivity stability measures) which will be integrated into smart farming applications in the field (e.g. fertilisation or precision farming) and will be compared to ground truth data like nitrogen sensor data, yield maps, or soil maps to evaluate their applicability.

2.3 Purpose of this Report

This report is the first step to setup the use cases. It reports on the detailed definition of the two use cases and summarizes the use case requirement. For the first use case, the particulate matter forecast service detailed in chapter two, this includes an introduction to the model to be used as well as the modes and additional modules which are planned to be used for the service operation.

The second use case, the Satellite Data Service for Agriculture (AgriCOpen), is outlined in chapter three. Here, the different data products to become available are defined and the workflow to obtain these data products from the input satellite data is shown. In addition, the tools to obtain the different products are defined.

3 Use Case I: PMFS – Particulate Matter Forecast Service

3.1 The WRF Model

The Weather Research and Forecast (WRF) model (Skamarock et al., 2008, Powers et al., 2017) is a state-of-the-art community forecast system developed for applications from climatological to micrometeorological applications. Furthermore, it serves research as well as operational purposes. The development is led by the National Centre for Atmospheric Research (NCAR) in Boulder, Colorado, and a large global community contributes new code developments. WRF has got almost 5000 registered users worldwide. The system quickly evolved during the last decade. The current version 4 is applied for the particulate matter forecast system in this project.

3.2 WRF-Chem and Large-Eddy simulation mode

From the core system, WRF has grown to provide several additional capabilities. For this project two of these additional modules are especially important, the in-line chemistry component WRF-Chem (Grell et al., 2005; Fast et al., 2006) and the so-called “Large-Eddy-Simulation” (LES)

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[3] https://luftdaten.info
[4] https://www.esa.int/Our_Activities/Observing_the_Earth/Copernicus/Sentinel-2

mode (e.g. Mirocha et al., 2010; Munoz-Esparza et al., 2014), allowing an explicit simulation of the larger part of the turbulence spectrum.

For the former, components for gas-phase and aqueous chemistry as well as the treatment of aerosols of different complexity are available, extending the applicability of WRF to a wide range of research applications in air chemistry ranging from dispersion modelling and air quality applications to basic research in aerosol-cloud-radiation interaction.

The LES mode applies a low-pass filter to split the equations into a resolved and a non-resolved part depending on the selected grid resolution. This allows the simulation of a large part of the turbulence evolving in the boundary layer explicitly, which is crucial for the prediction of chemical components and small-scale circulations in the boundary layers. Figure 1 shows an example of a simulation with 100 m resolution from an earlier project.

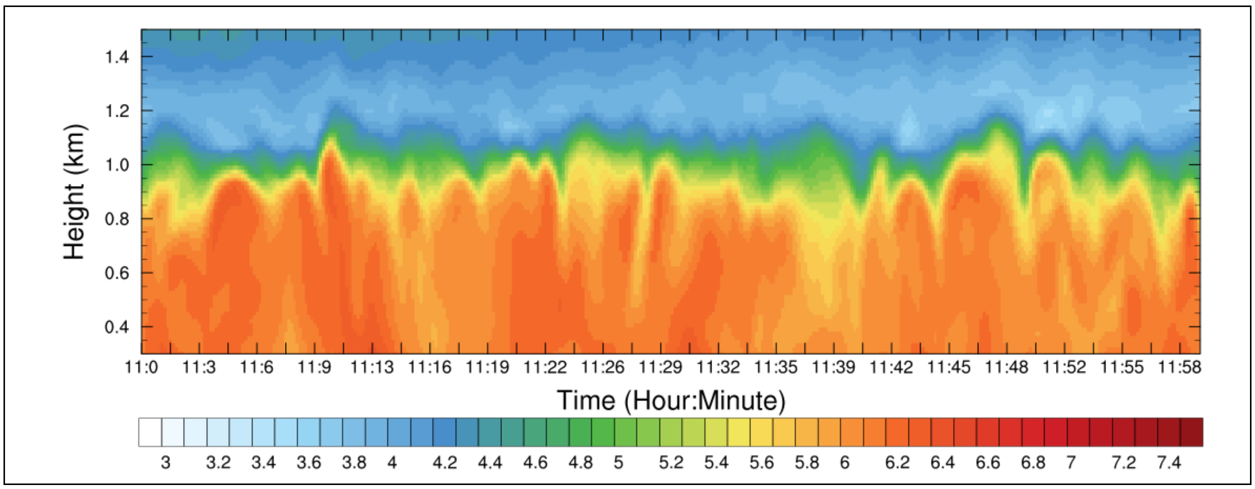

Figure 1: Development of turbulence in the boundary layer as simulated by WRF operated in LES mode. Shown is a time-height cross section of the water vapour mixing ratio (g/kg), illustrating the development of turbulent eddies in the boundary layer.

3.3 Set-up of the Particulate Matter Forecast System (PMFS)

The forecast system in this project is based on the WRF model system. A chain of three model simulations is set up ranging from a horizontal resolution of 1250m via 250m down to 50m horizontal resolution. In the vertical direction 100 levels up to a height of 50hPa (approximately 22km above sea level) are applied, at least 25 of them in the boundary layer. The depth of the vertical levels increases with height from about 50m in the boundary layer to 200m in higher levels. The meteorology is externally forced with analysis data from the European Centre for Medium Range Weather Forecasting (ECMWF[5]) and the three domains shown in Figure 2 are nested into each other. Communication between the nests is one-way, so the finer resolution is

[5] https://www.ecmwf.int

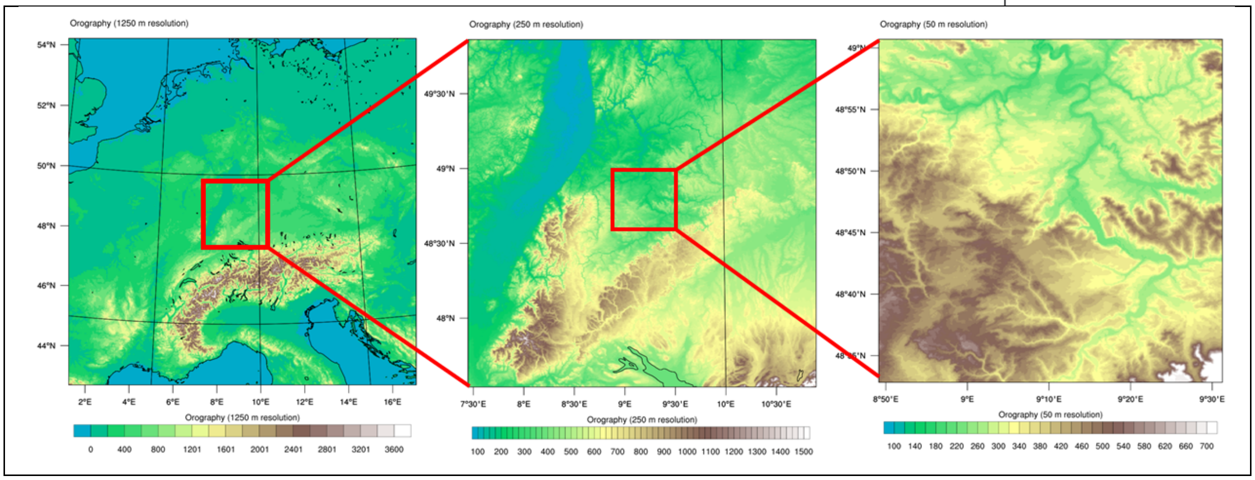

Figure 2: Domain configuration anticipated for the forecast system with 1250 m, 250 m and 50 m horizontal resolution.

driven by the coarser one without an information exchange backward from the finer to the coarser resolution. This allows direct comparisons of the performances of the different model resolutions.

Since the applied resolutions are not fine enough to resolve single buildings, the simulations include an urban canopy model to better represent the planetary boundary layer in urban areas. Figure 3 illustrates the processes taken into account for two different models available for WRF. The more sophisticated Building Effect Parameterization (BEM) is applied in this project.

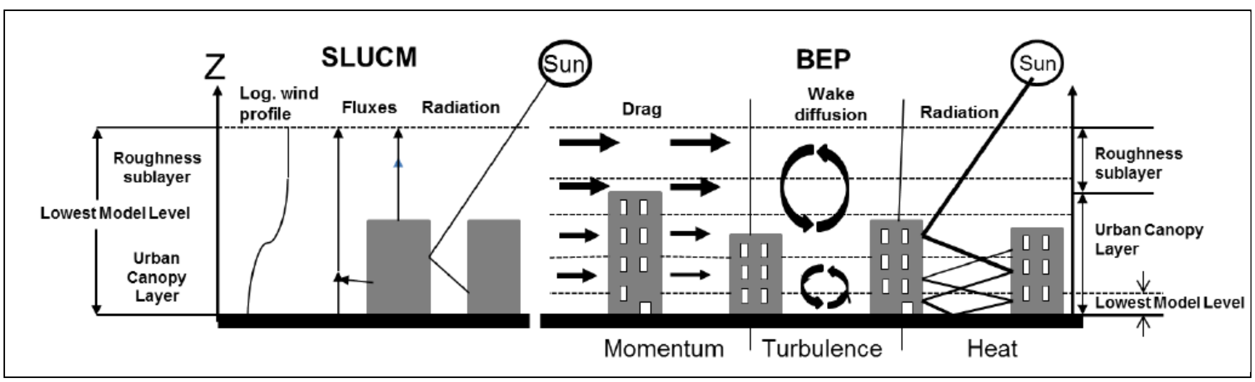

Figure 3: Schematic figure of the Single Layer Urban Canopy Model (Kusaka 2001) (left) and the multi-layer model: Building Effect Parameterization (Martilli 2002) right. These differ in representing the processes in the urban canopy layer (Chen 2011)

The chemistry is initialized by several steps. Data from global emission inventories provides the necessary background data in regions where no higher resolution observations are available. The data is processed by different chemical pre-processors and then integrated into the initial field from which the model forecasts are started. Furthermore, time and height varying input is provided from a chemical transport model (e.g. the MOZART model (Emmons et al., 2010) whose data can be downloaded from an archive). Finally, high-resolution emissions from European data bases and point observations are used to improve the initial field of the forecast. The whole process chain of the forecast system is illustrated in Figure 4.

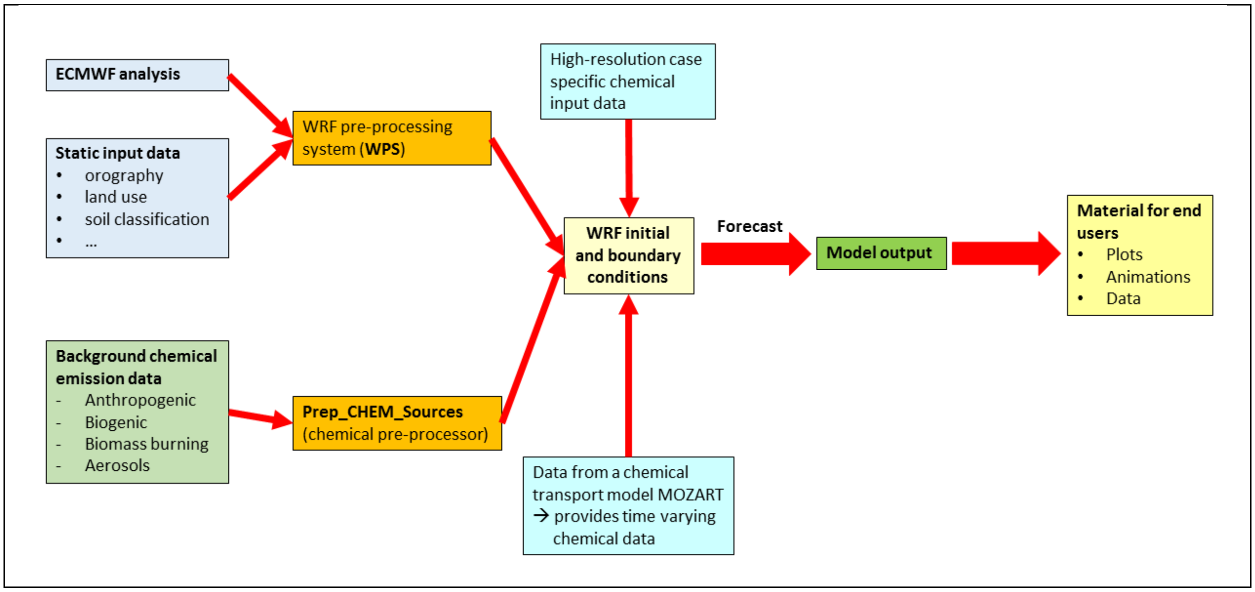

Figure 4: Set-up of the particulate matter forecast service

All preparation steps as well as the simulations and the subsequent post-processing of the data are done on the HLRS systems.

3.4 Status of the preparation of the Particulate Matter Forecast System

The WRF system version 4 including chemistry is compiled on the HLRS system. The configuration file for the urban canopy model is adjusted for Stuttgart following the work of Fallmann (2014) and the system is tested with the urban canopy model switched-on. The pre-processing tools for the global emission inventories are tested successfully on the HLRS system and the chemical pre-processing is done for a test case to solidify the necessary procedures.

Currently the first test of the model chain in the contemplated configuration is done. Here, tasks are to finally select the chemical components needed for the project (as sophisticated as necessary and as computationally efficient as possible) and estimate the needed amounts of computing time and storage for a typical test case. These tests provide the necessary numbers for the computing proposal to be written together with the other project partners.

Another important task at the moment is to find high-resolution emission data for Germany that will be used to most realistically initialize the simulations for the test cases. Here, we search for gridded inventory data on the km scale as well as point observations that can be used to densify the gridded data.

So far no decision about the cases selected for the demonstration of the forecast system is made. This strongly depends on the meteorological conditions as well as the available data for the initialization. The selection will be done in close cooperation with the other project partners as soon as the system itself is running properly on the HLRS system.

3.5 Software and IT requirements

The software necessary for the preparation of the initial fields as well as the forecasts is either open source (e.g. the WRF system and the pre- and post-processing tools) or provided by the HLRS computer system (e.g. compilers, debuggers …). While the pre-processing and post-processing of the initial, boundary and output data requires comparably small amounts of computing time and storage, WRF-Chem simulations themselves require a lot of computing time and storage space. Depending of the selected components up to more than 100 additional 4-D variables have to be calculated and stored. In terms of computing time simulations with WRF-CHEM need around 10 times more computing time compared to “meteorology-only” simulations. Final estimates for the needed amounts of computing time and storage cannot be provided before a complete test in the anticipated configuration is done on the HLRS system. This is work in progress at the moment. Therefore, first coarse estimates of the needed storage for one simulation, provided below, are derived from short tests done on an office PC for a small test domain.

<u>Storage needs for one case:</u>

One case is a simulation of two days with the anticipated domain configuration. In the outer two domains full meteorology is combined with an as simple as possible chemistry. In the inner domain full meteorology and sophisticated chemistry is applied. Interval with which model output is written is 30 min in the outer domain with 1250 m resolution, 10 min in the middle domain with 250 m and 5 min in the inner domain with 50 m resolution. Files to restart an interrupted simulation are written every hour in each domain. They are much larger than the model output files, but they can be deleted or even reduced in number after a successful simulation.

Table 1: Storage requirements of the use case

Domain (size of output file)	**Number of output files D01 (20 GB each)**	**Total storage for model output files**	**Number of restart files (3 to 4 times larger than the model output)**	**Total storage for restart files**	**Total storage needs**
D01 (20 GB)	96	1920 GB	48	3360 GB	5280 GB
D02 (20 GB)	288	5760 GB	48	3360 GB	9120 GB
D03 (65 GB)	576	37440 GB	48	12000 GB	49440 GB
Total sum					**63840 GB**

One case consumes 63 TB of disk space. This can be optimized by reducing the number of written model variables or by on-the-fly production of the needed plots with a subsequent deletion of the data.

The estimation of the needed computing time from results of smaller test cases done with different compilers on different platforms is not possible. The eye of the needle is the time needed to do file I/O. Corresponding numbers follow when the first test on the HLRS system is successfully finished.

4 Use Case II: AgriCOpen – Satellite Data Service for Agriculture

The goal of the AgriCOpen use case is the provision of products and services for agricultural smart farming practices based on open satellite imagery data of Sentinel-2. Digital agricultural practices need spatial information about the variability and current situation on agricultural fields to optimize management and production. Data analyses derive vegetation indices from satellite imagery, which are related to crop and soil parameters. These products can then be used to derive management zones for precision farming techniques or to estimate variations in yield potential or levels of fertilisation. The availability of specialized, ready-to-use satellite imagery products is a prerequisite for the integration into Farm Management Information Systems (FMIS). Such products foster the adoption of digital management practices and enable better decision making, as well as allow site-specific technology to be introduced on a larger scale.

The evaluation of workflows from satellite data to the defined products like mosaics, vegetation indices and zonal classifications will be conducted in close cooperation with end users (i.e. farmers) and within their IT-system structures. Timely processing is needed to process the data into products for the end-user. The integration of the HPC methods to deliver open data products are part of the proposed action as well as the offer of the generated products via standardized infrastructural components and interfaces, as there are the INSPIRE conform Web Map Service (WMS), Web Coverage Service (WCS) and Web Feature Service (WFS).

4.1 Workflow from satellite data to products

The workflow from satellite data to the products is depicted in Figure 1. In a first step, the Sentinel-2 1C-data will be downloaded via sentinel hub resp. CODE-DE platform and corrected for atmospheric influences to get Sentinel-2 2A-data. Alternatively, Sentinel-2 2A-data can be downloaded directly as a product. Depending on the usability of pre-computed 2A products and an internal evaluation of available processing options, it might be necessary to compute the 2A products with an adapted set of parameters (e.g. to correct the influence of clouds more specifically during Sen2Cor processing). As a next step a cloud mask is calculated, which on the one hand represents the basis for the indices calculation and on the other hand drives the mosaic calculation for each date the satellites passes over the area and for a 14 day period. Based on vegetation indices, the development of biomass over time can be taken into consideration for multitemporal analyses of the data. Finally a zonal classification can be generated on demand, which can either be based on the current situation and vegetation indices of recent dates or on long-term, multitemporal analysis results. Figure 5 gives an overview of the products processing chain, starting from downloading data to resulting, processed product types.

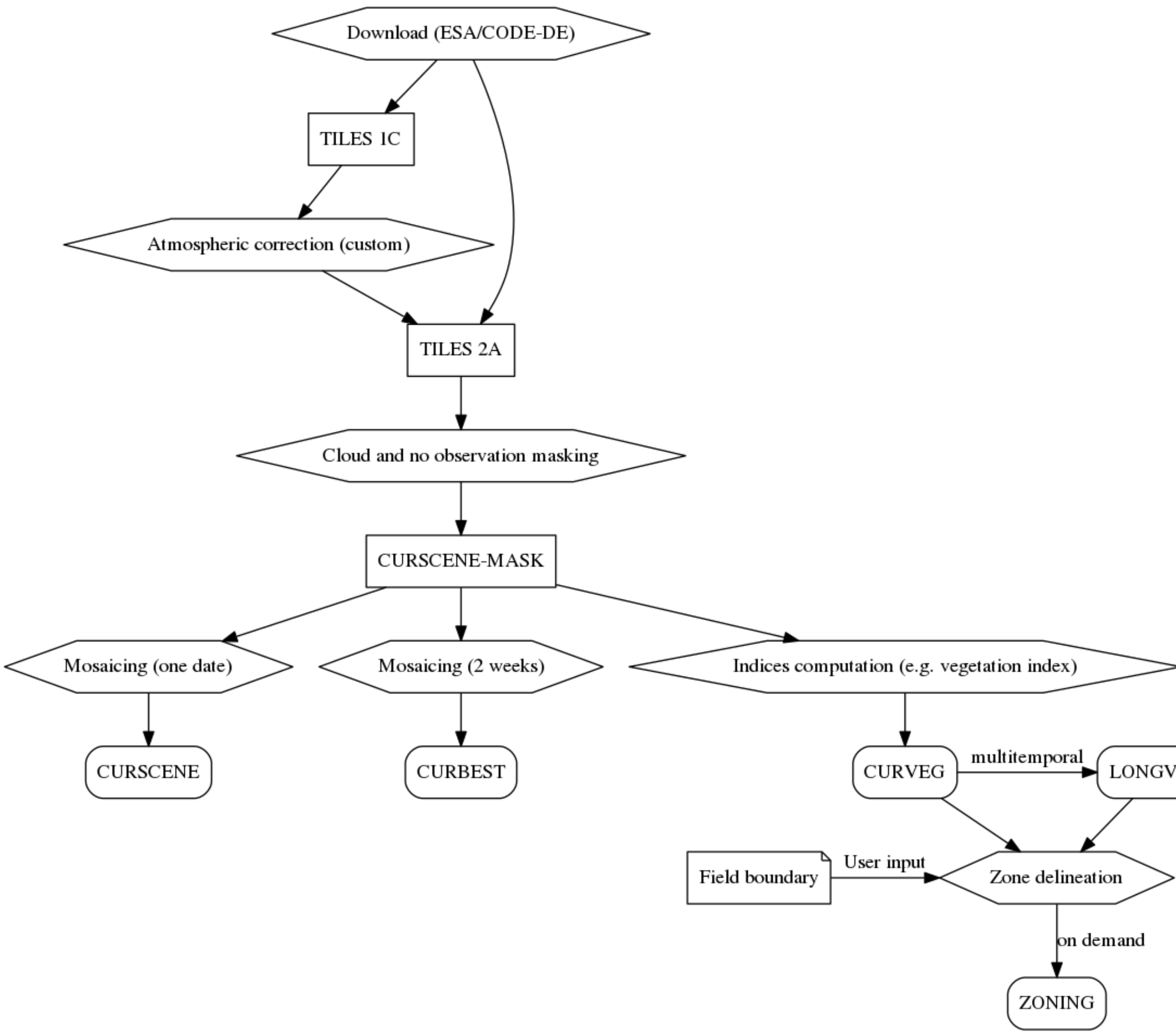

Figure 5: Workflow from satellite data to products: processing steps denoted by hexagons, boxes for products, products in rounded boxes will be publicly available.

4.2 Product definition

A total of seven products are defined, whereas only 4 products are intended to be provided for the user and one is computed on demand. The products and their derivation are described in the following.

4.2.1 Product: TILES

The first product (0) are the TILES of the Sentinel-2 measurement data, as they can be downloaded from the international Sentinel hub or the national CODE.DE portal for the area of Germany. Each tile covers an area of 100x100 km, and neighbouring tiles have an overlap.
The sentinel products are already processed to defined levels and can already include additional data layers like classification results. The following list denotes the processing levels of Sentinel-2 data acquired with the MSI instrument, according to the SENTINEL-2 User Handbook:

- Level-0, Level-1A and Level-1B products are not disseminated to users
- Level-1C: Top of atmosphere reflectances in fixed cartographic geometry, cloud and land/water masks are included
- Level-2A: Bottom of atmosphere reflectances in cartographic geometry, processed on the user side (e.g. Toolbox)
    - Scene Classification map (cloud, cloud shadows, vegetation, soils/deserts, water, snow, etc.) is included
    - operational product started May 2018 (on Sentinel hub)

The use case will start with products on level 2A or 1C. Level 2A is a relatively new product derived using a standard parameter set from 1C. It might be necessary to customize the parameters for the atmospheric correction in the use case, such that level 1C will be the starting point with customized derivation of level 2A. The main goal of a customization is to minimize the effect of cirrus clouds.
TILES are an internal product and not provided to the end users.

4.2.2 Product: CURSCENE-MASK

The second product are the Sentinel-2A data corrected for atmospheric influence, with additional masks for clouds (NODATA) and areas of no observation (NOOBS). The masks distinguish so-called “No Observation” areas (no measurements taken) and “No Data” areas (measured area, but unusable observations due to conditions, e.g. clouds). The resulting product is CURSCENE-MASK (current scene with masks derived).
It will be computed for Sentinel datatakes (observation stripes from arktis to antarktis) and limited to the region of Germany.
CURSCENE-MASK is also an internal product and not provided to the end users.

4.2.3 Products: CURSCENE and CURBEST

The next product level, which can be derived from CURSCE-MASK, are mosaics. Mosaics combine the data of one or more TILES to larger areas, either based on the swaths of the satellite measurements of one date or based on predefined regions (e.g. the area of Germany). The mosaics are updated either for each measurement and containing clouds where not avoidable. In overlapping areas the measurements can be selected according to the principle of minimum cloud coverage, best pixel and latest measured pixel (product 2.1 CURSCENE) or over a period of 14 days according to the principle last good pixel (product 2.2 CURBEST). The selection of pixels may be rule based, according to parameters like minimal cloudinesss, best pixel, latest observation.

CURSCENE is the product for further processing and both are suitable for visualization. For the end user CURBEST might be preferred as background layer in GIS or farm management (FMIS) applications due to its likely reduced cloud coverage.

4.2.4 Product: CURVEG

The products, derived in parallel to the mosaics, derive various indices based on the CURSCENE-MASK product. These indices are relevant for the agricultural domain: various indices have already been proposed and used. Certain indices can be used to derive biomass, fertilisation or yield levels. These are important to estimate general and small-scale differences of the vegetation status and are related to crop parameters.

Selection of possibly usable indices:

- NDVI: normalized differential vegetation index (from bands B04, B08)
- SAVI: soil adjusted vegetation index (based on B08, B04)
- EVI: enhanced vegetation index (based on B08, B04, B02)
- ARVI: Atmospherically Resistant Vegetation Index (based on B08, B04, B02)
- REIP: Red Edge Inflection Point (based on B04, B05, B06, B07)

The indices are computed per scene and for valid pixel measurements only, therefore the masked product will be taken as input. There are many more indices available to choose from, most of them can be found via Index DataBase (https://www.indexdatabase.de/db/is.php?sensor_id=96). The computation and usability of indices and derived products will be identified in other tasks (e.g. 2.2, 2.3, 5.4), and iterations will be necessary according to the progress and results of those tasks. For fertilisation tasks in agriculture, the REIP index of each Sentinel datatake should lead to valuable products for the delineation of management zones.

Also, the derived product LONGVEG might have certain requirements on the vegetation indices products and need to be taken into consideration.

4.2.5 Product: LONGVEG

The product LONGVEG will be calculated from CURVEG products over a period of time. The goal of the LONGVEG product is to provide spatially explicit differences in site conditions as a basis for the delineation of zones. Based on multitemporal data the product can be related to parameters like potential biomass, yield potentials or similar estimates. This product will be developed and further defined in iterations with other tasks.

4.2.6 Product: ZONING

The last product is a zonal classification which is computed on demand. For a delineation of zones field boundaries are necessary as input from the user, such that the computations yield the variability on comparable sites. Data of one or multiple fields can be analyzed, and result in a relative zoning, such that the given polygon areas are subdivided into possible management zones. This is a product for the end user, as site specific management can be based on the identified zones. The end user still has to decide about the variation, depending on the type of treatment and additional knowledge about the fields (e.g. sources of variability).

4.3 Software and IT requirements, OGC services

In this section details about the Software and IT requirements are given. The current planning status is based on several assumptions about the availability of access to upstream data (via data hubs) and the applicability of software. The estimation of computational requirements are based on the current state of planning and the defined region of interest (data sets are computed for the area of Germany). The computational effort cannot be detailed in the moment as the behavior of the intended applications on the HPC platform is currently unknown. Depending on the requirements of other tasks and the applicability of the products in practical evaluation there might be adaptations necessary to the workflow or details of the products. Therefore the current estimates will be refined as practical implementations exist and are executed.

4.3.1 TILES

Sentinel-2 1C and 2A data are preferably to be downloaded from CODE-DE hub due to high bandwidth connection between network of DLR and DMZ-HLRS. Access is planned via Calvalus Portal (https://processing.code-de.org/calvalus.jsp), download automation using the hub API (e.g. via https://github.com/olivierhagolle/Sentinel-download) or direct download of tiles via sentinelsat (https://github.com/ibamacrs/sentinelsat). Storage will be done locally on harddisk or magnetic band infrastructure.
There will be about 69 tiles necessary for the region of Germany. With a size of 600 MB per 1C tile the storage requirement adds up to 40 GB (per datatake). A slightly higher amount of data is expected for the level 2A tiles (800 MB per tile), adding up to about 55 GB. For this product there is an amount of nearly 100GB per satellite visit to be stored.

OGC services: none, the TILES product is internal and no OGC services created.

4.3.2 CURSCENE-MASK

Atmospheric correction of the 1C-data to level 2A can be computed via Sen2Cor software (http://step.esa.int/main/third-party-plugins-2/sen2cor/), ARCSI (https://www.arcsi.remotesensing.info/) or GRASS `i.atcor`. Advanced cloud masking is possible with algorithm implementations in fmask (http://pythonfmask.org/), GRASS, Sen2Agri, FORCE or MACCS. Masks with the values NODATA and NOOBS are created. These masks can later be applied to all bands. TILES are mosaiced to create the product CURSCENE-MASK containing data and masks. The CURSCENE-MASK product is internal and no public OGC services are provided.
The masks do not add considerable amounts of data (due to their compressibility). The resulting product therefore consist of the same amount of data as the TILES 2A product: 60 GB per scene.

OGC services: none

4.3.3 CURSCENE

For the creation of CURSCENE mosaicing of TILES with masks from CURSCENE-MASK will be done using Sen2Three, GRASS or gdal_merge. Additionally there is a need for automation of "best pixel" recognition and parallelization of computations for adjacent tiles (resulting pixel selections may be rule-based). The scene will be cut to the region of Germany – for one measurement date (datatake). The resulting product is suitable for visualization, therefore provided as WMS service. The product needs to be stored for further processing and the WMS service: estimated to 55 GB per scene.

OGC services: WMS

4.3.4 CURBEST

Similar to the processing of CURSCENE mosaicing of the TILES takes place using Sen2Three, GRASS or gdal_merge with a different "best pixel" recognition and selection. The product provides a best-pixel effort of a 14 day period, suitable for vizualization. Therefore a WMS service is provided publicly. The amount of data to be stored is about 165 GB for the 14 day period (three satellite visits/stripes). With each visit of a satellite the product gets updated (three updates per 14 days).

OGC services: WMS

4.3.5 CURVEG

Computations of the CURVEG product will be done using GRASS (function `i.mapcalc`) for selected vegetation indices. Since the indices are a central product, access via OGC services will be provided. They can be used for visualization purposes, therefore a WMS service is planned, and for computational usage and creation of derived products a WCS service will be provided. These sevices will be set up for a selected set of indices. For the derived products, e.g. LONGVEG, there may be more indices necessary internally, which are not necesssarily exposed as public service. Depending on the computational requirements for the index calculation these may be computed on demand. Thus the necessity to store the calculated indices data for each date may not be given. If data storage is necessary, about 5 GB per index and satellite visit is necessary. Depending on the amount of indices (about 10), this can add up to 50 GB per scene.

OGC services: WMS, WCS

4.3.6 LONGVEG

A multitemporal analysis of vegetation indices can be based on algorithms and models, which take the dynamic nature of vegetation development during vegetation periods into consideration. There are several software packages already freely available (e.g. TIMESAT, FORCE, SPIRIT). These need to be evaluated for their usability in the context of this task: availability of Sentinel-2 data processing, necessity and benefits of inclusion and combination with other satellite products (e.g. Landast, SPOT) and their applicability in an HPC context. Parts of the multitemporal computations are possible with GIS functionality (as provided by GRASS). Since this product is relevant for visualisazion and the creation of derived products at client side (end users), these products are provided both as WMS and WCS services.

OGC services: WMS, WCS

4.3.7 ZONING

Computation of management zones will be done using GRASS. Since a field boundary is needed as input, the computation has to be done on demand. The resulting data is a vector data layer with polygons for each management zone. Therefore a WFS service can be used to provide the resulting product. A solution for the user input needs to be created, this could either be implemented as a public WPS service interface or via a customized solution. It is possible, that the WFS with additional transactional part (WFS-T) can be used as input interface for the users data.

OGC service: WFS(-T), processing on demand

5 Acknowledgements

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