CAMS Service Evolution

D5.2. Implementation of the Flow of Agricultural Nitrogen (FAN)v2 model in SILAM

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1 Executive Summary

The FANv2 module has been extracted from the CESM, and its internal data structures were made independent from the Community Earth System Model (CESM) data storage classes.

The SILAM model has been updated adding extra functionalities required by the implementation of FANv2: explicit surface tiling, expansion of the soil humidity module, multi-layer structure of the soil description, creation of new quantities, and setting up new interfaces.

Particular challenges were faced in expansion of the soil humidity module, where several processes represented in CESM received very simplified loopbacks. More rigorous process descriptions will be put in place upon evaluation of possible options in external models and IFS-COMPO.

Key input datasets have been obtained in forms of semi-manually made maps.

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2 Introduction

2.1 Background

The European Union's flagship Space programme Copernicus provides a key service to the European society, turning investments in space-infrastructure into high-quality information products. The Copernicus Atmosphere Monitoring Service (CAMS, https://atmosphere.copernicus.eu) exploits the information content of Earth-Observation data to monitor the composition of the atmosphere. By combining satellite observations with numerical modelling by means of data assimilation and inversion techniques, CAMS provides in near-real time a wealth of information to answer questions related to air quality, climate change and air pollution and its mitigation, energy, agriculture, etc. CAMS provides both global atmospheric composition products, using the Integrated Forecasting System (IFS) of ECMWF - hereafter denoted the global production system -, and regional European products, provided by an ensemble of eleven regional models - the regional production system.

The CAMS AERosol Advancement (CAMAERA) project will provide strong improvements of the aerosol modelling capabilities of the regional and global systems, on the assimilation of new sources of data, and on a better representation of secondary aerosols and their precursor gases. In this way CAMAERA will enhance the quality of key products of the CAMS service and therefore help CAMS to better respond to user needs such as air pollutant monitoring, along with the fulfilment of sustainable development goals. To achieve this purpose CAMAERA will develop new prototype service elements of CAMS, beyond the current state-of-art. It will do so in very close collaboration with the CAMS service providers, as well as other tier-3 projects. In particular, CAMAERA will complement research topics addressed in CAMEO, which focuses on the preparation for novel satellite data, improvements of the data assimilation and inversion capabilities of the CAMS production system, and the provision of uncertainty information of CAMS products.

NH_3 emission from agriculture is the main source of this gas in the atmosphere, controlling formation of ammonium nitrate and thus affecting $PM_{2.5}$ aerosol concentrations. As a rule, NH_3 emission is estimated from statistical data at annual level and superimposed with seasonal profile obtained from observations of NH_3 in air. Such approach evidently misses all dynamics of the NH_3 emission and reduces the model skills on both NH_3 itself and NH_4NO_3 aerosols.

The motivation for the current development is to have the NH3 emission fluxes modelled online, explicitly handling the impact of meteorological conditions on the fluxes. This is in accordance with the overall SILAM strategy of shifting the priority from emission inventories towards emission modelling. Resolving the emission interactions with meteorological factors can bring a substantial improvement to the model skills, as demonstrated by the dynamic residential-heating simulations using the ambient temperature.

2.2 Scope of this deliverable

2.2.1 Objectives of this deliverable

This deliverable is the first step in implementation of the Flow of Agricultural Nitrogen (FAN) model v.2 in SILAM.

The FAN model (Vira et al., 2022) is a dynamic 1-D process model developed within the scope of the Community Earth System Model, CESM, and deeply embedded in its structures making development of the CESM-independent version and establishing the related SILAM interfaces highly demanding task. Therefore, the FAN implementation in SILAM have been distributed between the WP 5 and 6.

Objectives of WP 5 and WP 6 reflected in this deliverable and planned for the WP 6 report at M36 are as follows:

1. WP 5, D.5.2, M18
    a. Detach the model from CESM and implement a more generic interface for coupling with SILAM and other models (this deliverable).
    b. Create necessary intermediate structures and models present in CESM but not suitable for up-taking into SILAM, first of all, processes related to soil humidity and water pathways underground.
    c. Collect updated input data as needed: currently in 0.5-degree maps, most of these data are based on sources available with a higher resolution (this deliverable).
2. WP 6, M36
    a. Test and refine the FAN implementation in SILAM, reproduce the results presented by (Vira et al., 2022) with SILAM computations, secure technically working and efficient model code
    b. Improve FAN version of SILAM by adjusting the seasonal and spatial variability via a more realistic representation of fertilization practices
    c. Evaluate the obtained implementation against CESM results, existing regional inventories, and atmospheric observations.

For WP 5, it is sufficient to reproduce the input data at the FAN v2 resolution, not going back to original datasets and repeating the compilation.

2.2.2 Work performed in this deliverable

In this deliverable the work as planned in the Description of Action (DoA, WP5 T5.2) has been performed.

Technical details of the implementation work are described in the next sections. In-short, the following steps have been performed.

1. The FAN code was extracted from the CESM distribution package as two modules: FAN itself and its interface to the upper-level driver.
2. The dependencies on the underlying classes and objects, which are embedded in FAN interface and only partly encapsulated, have been cut and documented for the following replacement with the corresponding SILAM variables
3. The SILAM code and hierarchy of classes was examined for missing variables, classes, processes, and modules. This step was repeated several times iteratively during the further work, which revealed several layers of such dependencies.
4. Missing variables have been created and connected to the main SILAM structures
5. Two most-important updates of the SILAM structure were:
    a. Introduction of the surface tiling, the definition of the corresponding new class and minimal set of procedures connecting it to other parts of the model
    b. Expansion of the soil description to a multitude of layers. For FANv2, two layers was sufficient, but a possibility of more layers has been created if, e.g., elements of VIC soil moisture model are eventually added (VIC uses three layers).
6. Other missing classes and process models have been created, updated, or patched with place-holders mimicking the behaviour of the target structures. The most-important patch referred to soil water processes.
7. SILAM structures and classes for surface description were updated and expanded to cover the needs of FAN

8. FAN interface to the CESM land model has been rewritten completely and simplified to allow for plugging the module to SILAM updated structure.
9. FAN interface to the CESM soil water model has been patched with highly simplified surrogates mimicking the data flows of the VIC soil water model, maintaining qualitatively the same range of variables and similar monotonicity of the response. A rigorous solution for the soil water modelling was left to the WP 6 as it requires a substantial expansion of the SILAM soil water module and alignment with ECLand to simplify the potential application of the model in the IFS-COMPO.
10. The code has been preliminarily cross-checked for harmonized units, physical meaning of variables, their dimensions, input and output. More detailed checks will be performed during the testing phase in WP 6.

2.2.3 Deviations and counter measures

No significant deviations have been encountered.

2.2.4 CAMAERA Project Partners:

HYGEOS	HYGEOS SARL
ECMWF	EUROPEAN CENTRE FOR MEDIUM-RANGE WEATHER FORECASTS
Met Norway	METEOROLOGISK INSTITUTT
RC.io	RESEARCHCONCEPTS IO
BSC	BARCELONA SUPERCOMPUTING CENTER-CENTRO NACIONAL DE SUPERCOMPUTACION
KNMI	KONINKLIJK NEDERLANDS METEOROLOGISCH INSTITUUT-KNMi
SMHI	SVERIGES METEOROLOGISKA OCH HYDROLOGISKA INSTITUT
FMI	ILMATIETEEN LAITOS
MF	METEO-FRANCE
TNO	NEDERLANDSE ORGANISATIE VOOR TOEGEPAST NATUURWETENSCHAPPELIJK ONDERZOEK TNO
INERIS	INSTITUT NATIONAL DE L ENVIRONNEMENT INDUSTRIEL ET DES RISQUES - INERIS
IOS-PIB	INSTYTUT OCHRONY SRODOWISKA - PANSTWOWY INSTYTUT BADAWCZY
FZJ	FORSCHUNGSZENTRUM JULICH GMBH
AU	AARHUS UNIVERSITET
ENEA	AGENZIA NAZIONALE PER LE NUOVE TECNOLOGIE, L'ENERGIA E LO SVILUPPO ECONOMICO SOSTENIBILE

3 Technical implementation

3.1 FAN core modules that have been adopted as-is or close to that

FAN is based on a comprehensive resistance analogy that describes the exchange of N-containing components (Figure 1). The key processes include: bi-directional exchange of NH3 between soil and the atmosphere, phase transition between aqueous and gaseous phases, soil run-off and long-term fixation in deep layers.

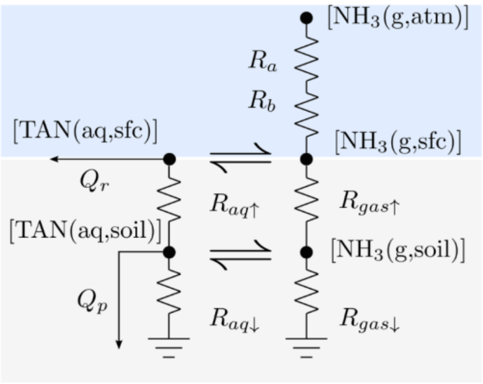


Figure 1. Baseline resistance scheme for NH3 exchange between the FAN compartments. Adopted from (Vira et al., 2022)

The Figure 1 reveals the first roadblock. FAN is deeply embedded into CESM and closely interacts with the soil humidity model, which is a separate module of CESM, in turn deeply integrated with other modules describing soil and atmospheric processes. The corresponding soil humidity processes are described by the Variable Infiltration Capacity, VIC, model (Hamman et al., 2018). FAN uses several variables calculated by VIC but does not return the information into VIC, thus using it as an external driver and allowing, in principle, a one-way implementation of the data flow. In particular, VIC model can be embedded in SILAM: VIC is an open-code system with comparatively detailed documentation. However, the VIC model by far exceeds the needs and level of details of the surface process description in SILAM. Secondly, VIC may be not compatible with IFS ECLand system. Finally, VIC by far exceeds the needs of FAN, being itself many times larger than FAN. Therefore, the full implementation of VIC just for driving the FAN soil processes is a clear overshot.

Another fundamental principle of FAN is its multi-pool structure (Figure 2). It allows for representation of a gradual ageing and NH_3 release of the N-containing compounds introduced into the soil via different pathways.

The multi-pool structure of Figure 2 highlights the second major dependence of FAN on the underlying model: the multitude of land uses considered by FAN but controlled by the surface modules of CESM. In particular, CESM distinguishes 4 layers of the soil class hierarchy: Gridcell, Landunit, Column, and Patch (Figure 3). These classes are directly related to various processes considered by CESM and form a backbone of CESM calculations. The SILAM surface-related structures are completely different and much simpler. In particular, until now SILAM does not use subgrid tiling. Therefore, maintaining the CESM surface hierarchy is neither feasible nor necessary for FAN operations inside SILAM.

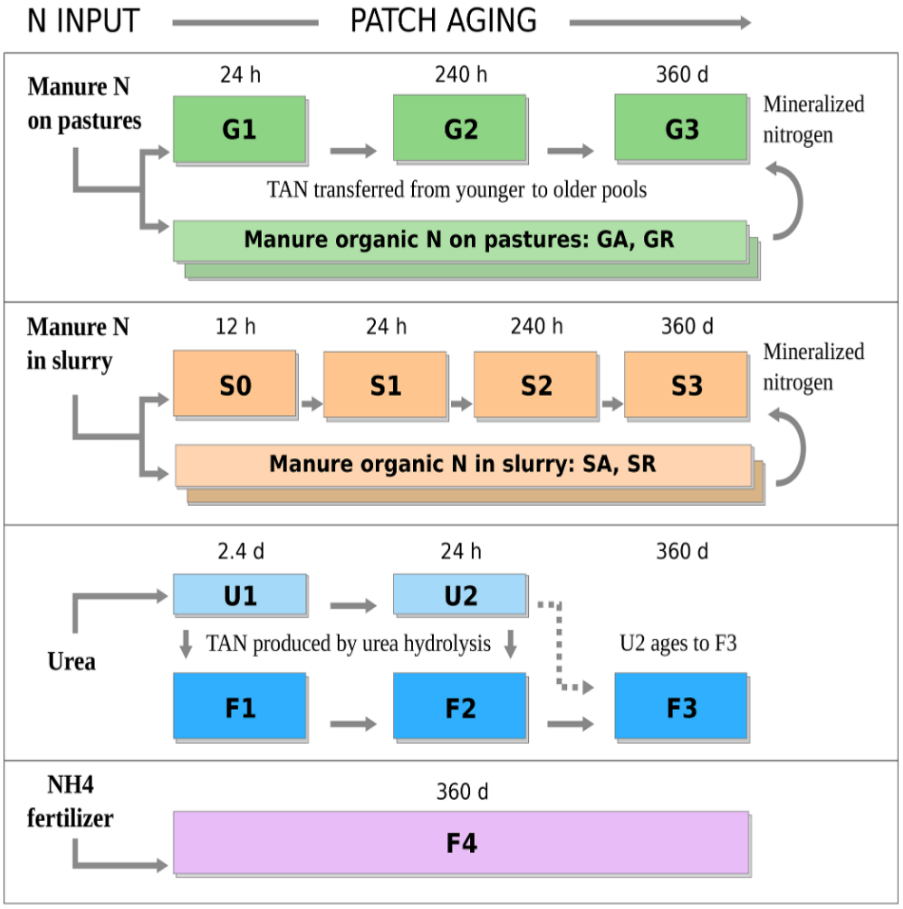


Figure 2. Multi-pool structure of FANv2. Adopted from (Vira et al., 2022)

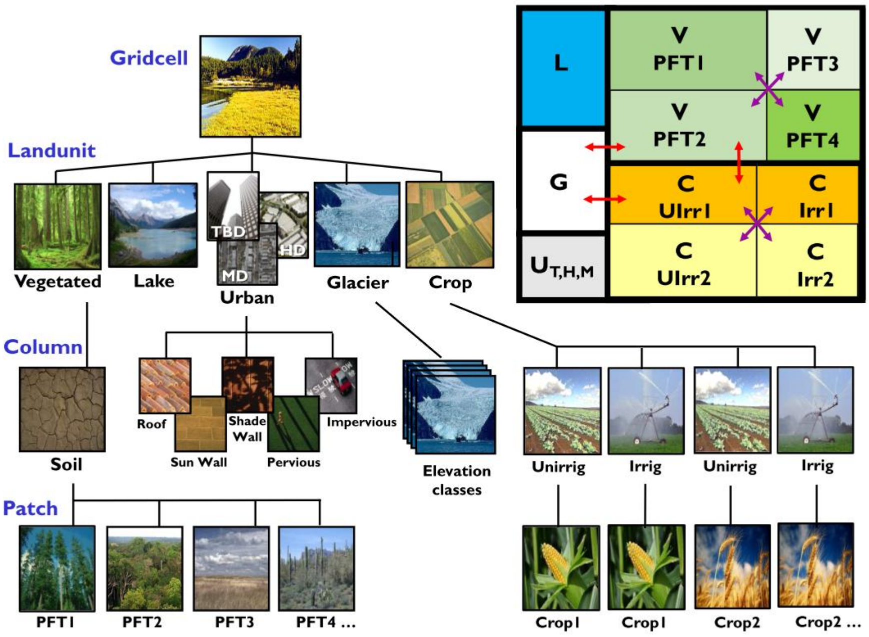


Figure 3. Land surface classes in CESM surface description.

3.2 Surface classes of CESM, FAN, and SILAM

FAN is formally built at the level of Columns but interacts with several other levels. It uses only a subset of the surface classes of CESM (Figure 3):

- The Soil Column taken as an equivalent of wild vegetation since this Column is the only one in the Vegetated Landunit
- The Crop Landunit taken as a Crop Column, whether irrigated or not
- All other Columns are ignored and jumped over in the calculations.

SILAM baseline surface description relies on integrated characteristics calculated at the start of the simulations. The static parameters are fraction of land, fraction of water, fraction of low and high vegetation, etc. They were not considered as a model-wide set of tiles, such term was never used in SILAM. The sum of fractions is not bound to unity and can be both smaller and larger than 1.0. Each physical module operated with the corresponding type of the surface accounting for its actual area in the grid cell and computes area-integrable variables. For instance, emission of sea salt is computed for grid cells with the water area exceeding 0.1% of the grid cell – and the total flux is the integrable output variable, taken proportional to the grid cell area multiplied with the water area fraction. The approach provides very high flexibility, essentially allowing individual physical modules to operate each in its own convenient phase space and use convenient variables. The limitation is also evident: in absence of formally defined tiles, exchange between them could not be defined.

Incorporation of FAN forced the major update in SILAM: introduction of subgrid tiles. It allowed for a straightforward mapping of the FAN processes of Figure 1 and Figure 2. Seizing the chance, definition of the tiles was aligned with vegetation classes used by the SILAM fire subsystem in connection with the IS4FIRES global fire information system. In the end, the list of tile types has been set (for now) as follows:

```
INTEGER, PARAMETER, PUBLIC :: fraction_of_ice_flag = 250026
INTEGER, PARAMETER, PUBLIC :: fraction_of_land_flag = 250027
INTEGER, PARAMETER, PUBLIC :: fraction_of_water_flag = 250028
INTEGER, PARAMETER, PUBLIC :: fraction_of_forest_flag = 250029
INTEGER, PARAMETER, PUBLIC :: fraction_of_erodible_soil_flag = 250030
INTEGER, PARAMETER, PUBLIC :: fraction_hv_flag = 250051
INTEGER, PARAMETER, PUBLIC :: fraction_lv_flag = 250052
integer, parameter, public :: fraction_of_vegetatedland_flag = 250214
integer, parameter, public :: fraction_of_forest_flag = 250215
integer, parameter, public :: fraction_of_shrub_flag = 250216
integer, parameter, public :: fraction_of_crop_flag = 250217
integer, parameter, public :: fraction_of_grass_flag = 250218
integer, parameter, public :: fraction_of_boreal_forest_flag = 250219
integer, parameter, public :: fraction_of_temperate_forest_flag = 250220
integer, parameter, public :: fraction_of_tropical_forest_flag = 250221
integer, parameter, public :: fraction_of_polar_shrub_flag = 250222
integer, parameter, public :: fraction_of_nonpolar_shrub_flag = 250223
```

Maintaining the SILAM flexibility, most of fractions can be combined in a random order, and their sum is not bound to unity. The specific list of tiles is identified at the start of the run and depends on the physical modules involved. FAN needs fraction_of_crop_flag and fraction_of_grass_flag, whereas the rest of the vegetated area of grid cells is represented by fraction_of_forest_flag and fraction_of_shrub_flag. Within the SILAM FAN module, non-vegetated parts of grid cells are ignored, similar to the original FAN.

3.3 Update of the soil water model

As pointed out above, the VIC model used in CESM is too large and too complicated for the purposes of FAN-SILAM calculations. However, some elements of it were needed and, being comparatively well isolated, have been introduced in SILAM water_content_in_soil module.

The key starting point was the classical empirical parameterization of soil properties as functions of soil type (Clapp and Hornberger, 1978). FAN and CESM use the relations as lookup tables. However, a simple analysis showed that the semi-qualitative table naming soil types one-by-one is almost entirely irrelevant. As seen in Figure 4, a vast majority of parameters demonstrate nearly perfect linear (or hyperbolic) relations. FAN needed the b and ψ coefficients, both very convincingly reproduced via regression equations. The corresponding subroutine has been implemented in water_content_in_soil module of SILAM

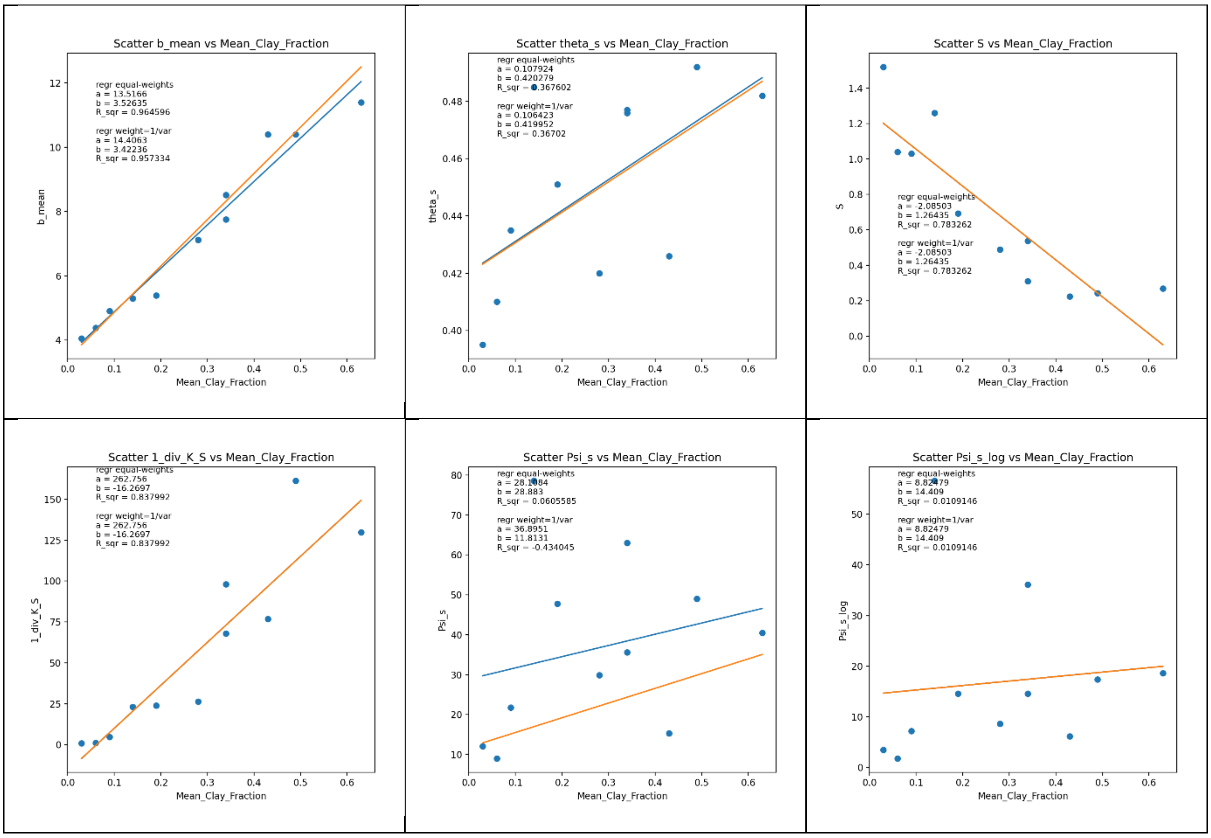


Figure 4. Scatterplots and regression relations for the look-up tables of (Clapp and Hornberger, 1978)

3.4 Interface FAN-SILAM

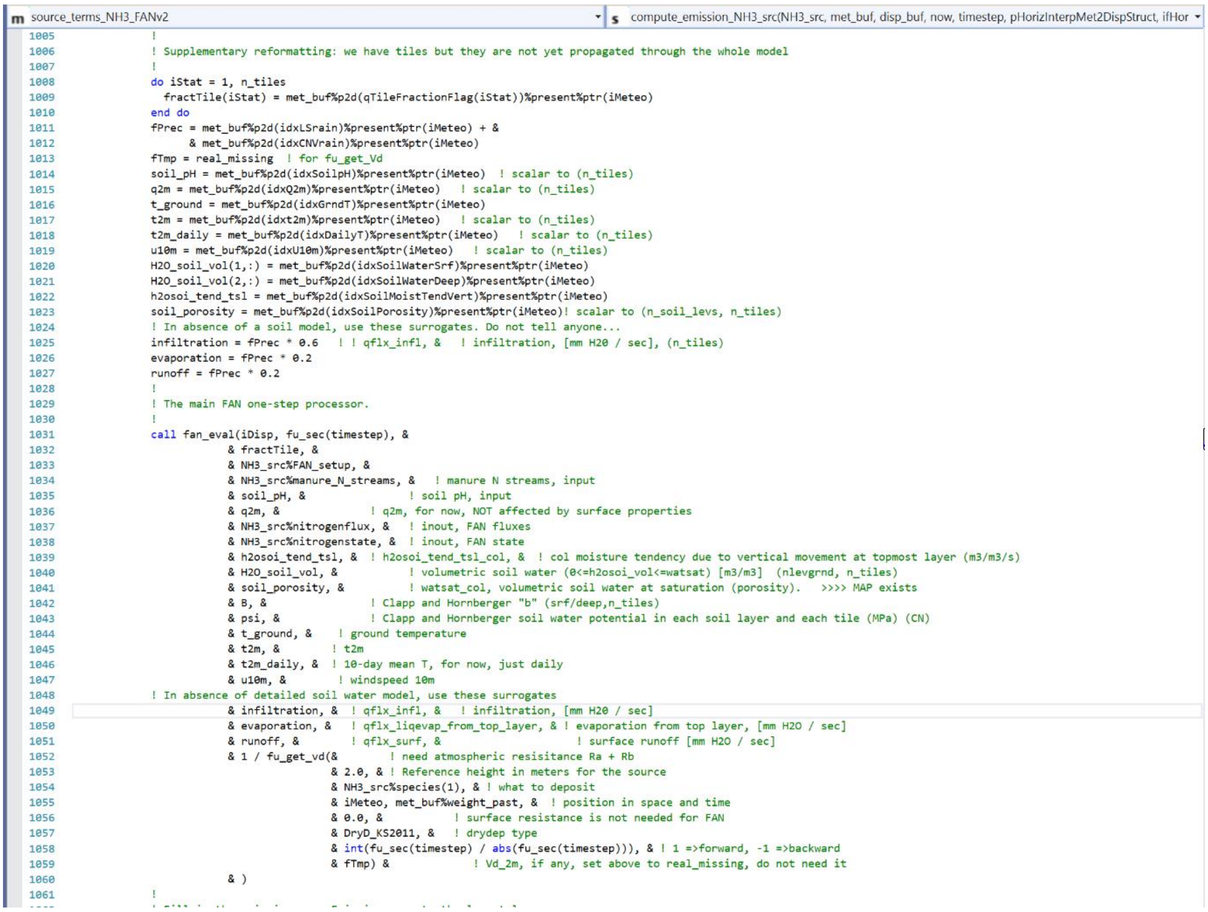
Upon expansion of SILAM and introduction of the tiling concept, the interface for FAN has become comparatively straightforward. It started from the new NH3 source term formulated in a similar manner as all source terms of SILAM (Table 1).

The key functionality of FAN interface is implemented via the subroutine fan_eval, which is called from the compute_emission_NH3_src subroutine. Its analogy exists in the original code, but heavily uses the CESM classes and data structures. Therefore, it has been largely rewritten, still maintaining the FAN call as tightly as possible: except for the Column to tiles conversion, rest of the FAN call remained practically unchanged (Figure 5).

Apart from the fan_eval, the initial code includes budget calculations and sanity checking subroutines. They have been adapted accordingly.

Table 1. Content of the top-level interface for the new NH3 source

Source_terms_NH3_FANv2,		New module
public	fill_NH3_src_from_namelist.	Reading the source features and input file locations from an input namelist.
public	reserve_NH3_source	Reserves space for the NH3 source in SILAM source list
public	init_emission_NH3	Initialises internal fields of the source, including FAN variables and input fields
public	create_source_containing_grid	Creates a grid that covers the source area (mandatory item in SILAM, trivial for global sources)
public	source_2_second_grid	Projects the source and its internal fields to a second grid provided as an input
public	add_source_species_NH3_src	Registers NH3 species released by the source into the list of emitted species
public	add_input_needs	Creates a list of meteorological and physiographic quantities needed for FANv2 operations
public	link_source_to_species	Sets mapping between the NH3 source and the main data pools of the run
public	prepare_inject_NH3_src	Intermediate steps resetting pointer to dynamic meteorological fields at each time step
public	compute_emission_NH3_src	Main subroutine computing NH3 emission for one time step
public	fu_NH3_emis_owned_quantity	Encapsulation functionality
public	fu_name	Encapsulation functionality
public	fu_source_nbr	Encapsulation functionality
public	fu_source_id_nbr	Encapsulation functionality
public	fu_species	Encapsulation functionality
public	typical_species_conc	Encapsulation functionality
public	Report	Reports the setup of the source


m source_terms_NH3_FANv2
s compute_emission_NH3_src(NH3_src, met_buf, disp_buf, now, timestep, pHorizInterpMet2DispStruct, ifHor

```
            !
            ! Supplementary reformatting: we have tiles but they are not yet propagated through the whole model
            !
            do iStat = 1, n_tiles
              fractTile(iStat) = met_buf%p2d(qTileFractionFlag(iStat))%present%ptr(iMeteo)
            end do
            fPrec = met_buf%p2d(idxLSrain)%present%ptr(iMeteo) + &
                  & met_buf%p2d(idxCNVrain)%present%ptr(iMeteo)
            fTmp = real_missing  ! for fu_get_Vd
            soil_pH = met_buf%p2d(idxSoilpH)%present%ptr(iMeteo)  ! scalar to (n_tiles)
            q2m = met_buf%p2d(idxQ2m)%present%ptr(iMeteo)   ! scalar to (n_tiles)
            t_ground = met_buf%p2d(idxGrndT)%present%ptr(iMeteo)
            t2m = met_buf%p2d(idxt2m)%present%ptr(iMeteo)   ! scalar to (n_tiles)
            t2m_daily = met_buf%p2d(idxDailyT)%present%ptr(iMeteo)   ! scalar to (n_tiles)
            u10m = met_buf%p2d(idxU10m)%present%ptr(iMeteo)   ! scalar to (n_tiles)
            H2O_soil_vol(1,:) = met_buf%p2d(idxSoilWaterSrf)%present%ptr(iMeteo)
            H2O_soil_vol(2,:) = met_buf%p2d(idxSoilWaterDeep)%present%ptr(iMeteo)
            h2osoi_tend_tsl = met_buf%p2d(idxSoilMoistTendVert)%present%ptr(iMeteo)
            soil_porosity = met_buf%p2d(idxSoilPorosity)%present%ptr(iMeteo)! scalar to (n_soil_levs, n_tiles)
            ! In absence of a soil model, use these surrogates. Do not tell anyone...
            infiltration = fPrec * 0.6   ! ! qflx_infl, &   ! infiltration, [mm H20 / sec], (n_tiles)
            evaporation = fPrec * 0.2
            runoff = fPrec * 0.2
            !
            ! The main FAN one-step processor.
            !
            call fan_eval(iDisp, fu_sec(timestep), &
                        & fractTile, &
                        & NH3_src%FAN_setup, &
                        & NH3_src%manure_N_streams, &   ! manure N streams, input
                        & soil_pH, &                ! soil pH, input
                        & q2m, &              ! q2m, for now, NOT affected by surface properties
                        & NH3_src%nitrogenflux, &   ! inout, FAN fluxes
                        & NH3_src%nitrogenstate, &  ! inout, FAN state
                        & h2osoi_tend_tsl, &  ! h2osoi_tend_tsl_col, &  ! col moisture tendency due to vertical movement at topmost layer (m3/m3/s)
                        & H2O_soil_vol, &           ! volumetric soil water (0<=h2osoi_vol<=watsat) [m3/m3]  (nlevgrnd, n_tiles)
                        & soil_porosity, &          ! watsat_col, volumetric soil water at saturation (porosity).   >>>> MAP exists
                        & B, &                ! Clapp and Hornberger "b" (srf/deep,n_tiles)
                        & psi, &              ! Clapp and Hornberger soil water potential in each soil layer and each tile (MPa) (CN)
                        & t_ground, &    ! ground temperature
                        & t2m, &        ! t2m
                        & t2m_daily, &  ! 10-day mean T, for now, just daily
                        & u10m, &        ! windspeed 10m
            ! In absence of detailed soil water model, use these surrogates
                        & infiltration, &  ! qflx_infl, &   ! infiltration, [mm H20 / sec]
                        & evaporation, &   ! qflx_liqevap_from_top_layer, & ! evaporation from top layer, [mm H2O / sec]
                        & runoff, &        ! qflx_surf, &                  ! surface runoff [mm H2O / sec]
                        & 1 / fu_get_vd(&        ! need atmospheric resisitance Ra + Rb
                                & 2.0, & ! Reference height in meters for the source
                                & NH3_src%species(1), & ! what to deposit
                                & iMeteo, met_buf%weight_past, &  ! position in space and time
                                & 0.0, &           ! surface resistance is not needed for FAN
                                & DryD_KS2011, &   ! drydep type
                                & int(fu_sec(timestep) / abs(fu_sec(timestep))), & ! 1 =>forward, -1 =>backward
                                & fTmp) &            ! Vd_2m, if any, set above to real_missing, do not need it
                        & )
            !
```

Figure 5. A screenshot of the new form of the fan_eval call.

4 Parallelization

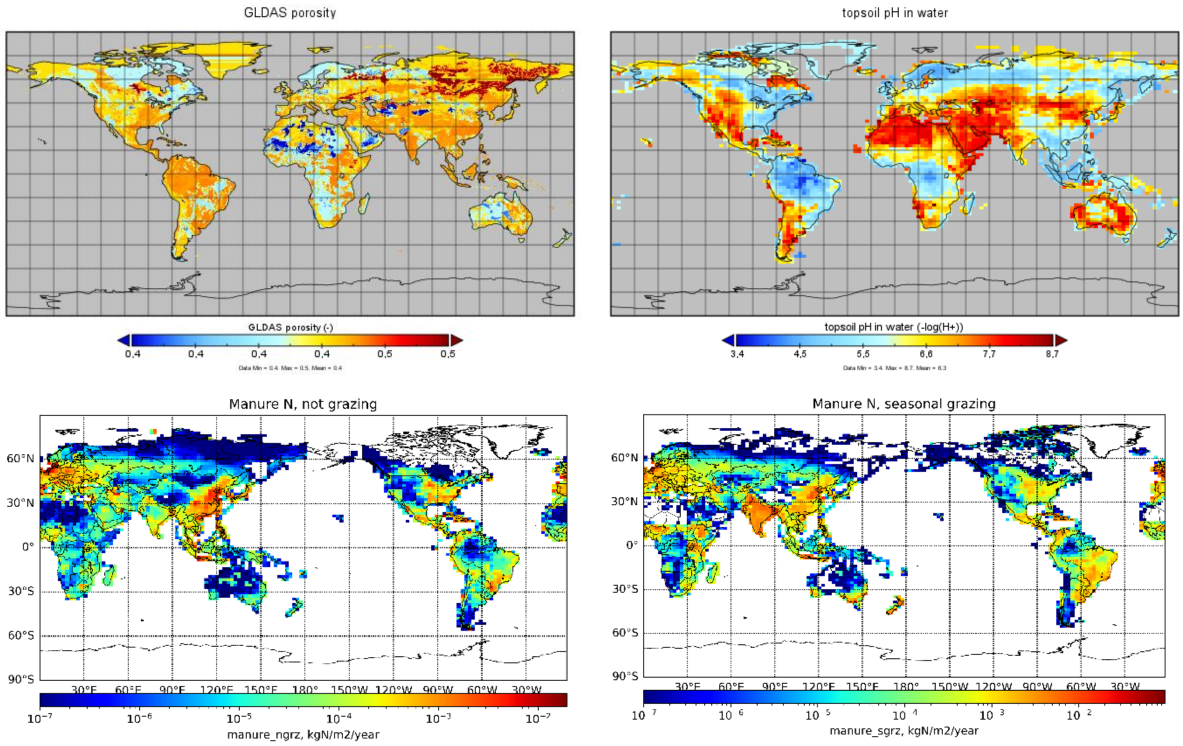
SILAM is a extremely heavily parallelized model. It follows the hybrid paradigm, where MPI and OMP approaches are applied simultaneously. As a result, global applications can easily employ 3-4 thousand cores with additional hyperthreading. Further scaling is usually hampered by the Infiniband connections between the nodes of supercomputers.

The MPI parallelization is applied so that the individual processes are given their own domains and grids to handle, so that the low-level routines, including source terms, are completely unaware about other domains. Since FAN was wrapped into the standard SILAM source term module, this parallelization should not notice the additional model.

The OMP (aca shared-memory) parallelization is not so simple in implementation. It is usually implemented via parallel blocks explicitly isolated within the code and parallelized cycles of the grid within those. To facilitate this parallelization for FAN, its governing subroutine, fan_eval, has been additionally modified so that it no longer scans the whole grid, instead handling only one grid cell. The domain scan is left to upper modules, which are SILAM native. Since grid cells do not interact with each other, this approach allows for eventual OMP parallelization. The decision of its necessity will be taken once the debugging of the system is finished and its runtime assessed.

5 Input datasets

FANv2 includes several datasets, which describe the relevant processes, in form of static maps. These were complemented with the clay fraction from the ECOCLIMAP dataset reflecting the newly found parameterization of the soil properties as functions of the clay fraction (Figure 4). A few examples are collected at the Figure 6.



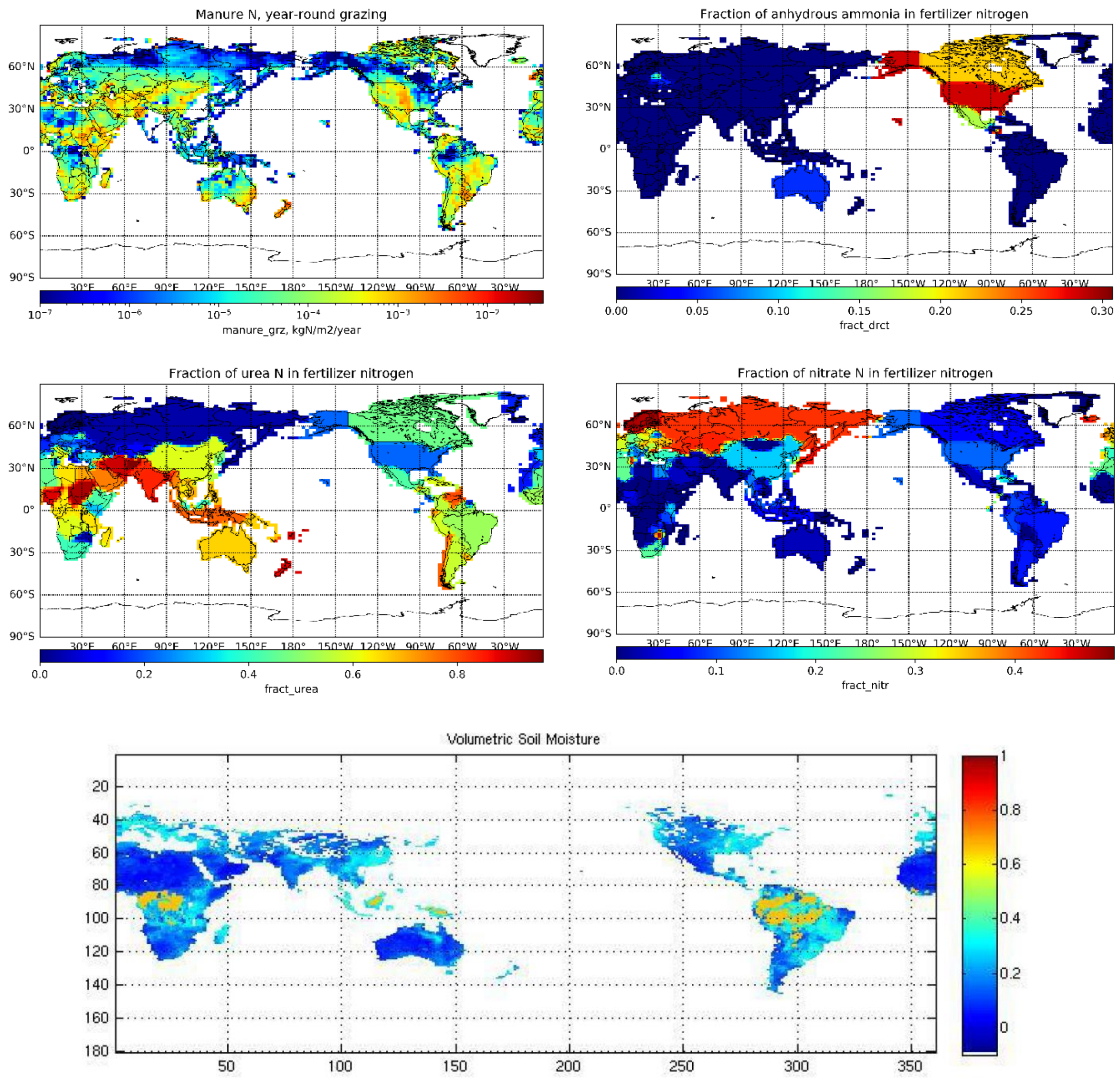


Figure 6. Examples of maps needed by FANv2.

6 Conclusions

This Deliverable described the measures and technicalities of the FANv2 implementation in SILAM, keeping in mind its potential further uptake by the IFS-COMPO.

The FANv2 module has been extracted from CESM, and its internal data structures were made independent from the CESM data storage classes.

SILAM model has been updated adding extra functionality: explicit surface tiling, expansion of the soil humidity module, multi-layer structure of the soil description, creation of new quantities, and setting up new interfaces.

Particular challenges were faced in expansion of the soil humidity module, where several processes represented by VIC model in CESM received very simplified loopbacks. More rigorous process descriptions will be put in place upon evaluation of possible options in external models and IFS-COMPO.

Key input datasets have been obtained in forms of semi-manually made maps.

Document History

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Internal Review History

Internal Reviewers	Date	Comments

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