Project: bm1400
Project title: Integriertes Treibhausgase-Monitoringsystem für Deutschland (ITMS)
Principal investigator: Dr. habil. Christoph Gerbig
Allocation period: 2024-01-01 to 2024-10-30

Achievements during the previous allocation period (01/2024 to 10/2024)

Computation time and disc space: The achievements with the HLRE platform during the previous allocation are reported as follows:

Module M:

-CSR + STILT (0.25 x 0.25 degrees): Biogenic CO_2 flux estimates are calculated using CSR with STILT (0.25 x 0.25 degrees) over the domain of Europe for 2006-2023. The spatial distributions of 2023 flux estimates show that the European domain is a weaker sink of CO_2 than suggested by the prior biosphere model VPRM (Figure 1). The inversion estimates are guided by the atmospheric observations collected from 59 in situ stations (ICOS and non-ICOS) distributed all over Europe.

In addition to the CO_2 and CH_4 inversions, the CSR system has also been used to evaluate process-based radon (Rn) flux maps by performing a Rn inversion for the year 2021 (Figure 2). Moreover, a dual-tracer CH_4-Rn inversion has been set up within the CSR framework and first test runs have been performed for the year 2021. Currently, the CH_4-Rn inversion only covers a single year for testing of the approach, and for assessing its potential to improve CH_4 emission estimates. In future this will be expanded to multiple years, utilizing all Rn observations.

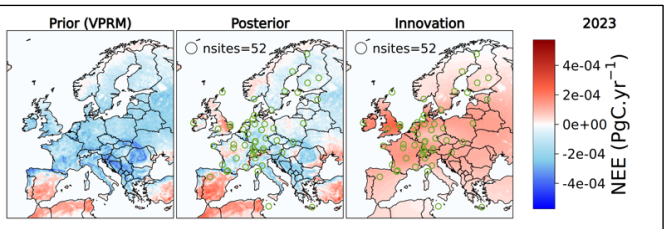

Figure 1: *Prior CO_2 fluxes calculated with the biosphere model VPRM (left), posterior fluxes estimated using CSR (middle), Innovation of fluxes (posterior – prior, right).*

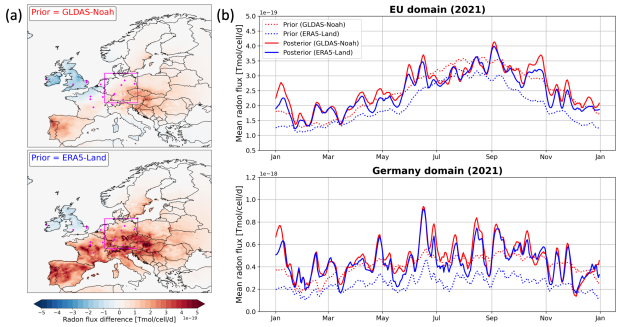

Figure 2: *Results of the Rn inversion: The a-posteriori fluxes are larger and show higher temporal variability than the process-based a-priori Rn fluxes in Germany in 2021.*

-ICON-ART - CTDAS (R3B08, 6.5 km resolution): After the previously successful synthetic experiment of inversions using ICON-ART–CTDAS with pseudo observations, we attempted to assimilate actual satellite XCH_4 data from the TROPOMI WFMD product. Within Europe, a total of 944,845 satellite observations over the course of 30 days were assimilated, aiming to provide CH_4 emission estimates for June 2018 (Figure 3). In order to work with the EnKF-based inversion system CTDAS, a configuration of ensemble simulations carrying 100 tracers needed to be carried out. This required significant resources from Levante for both computational and storage. However, with the initial attempt to assimilate real data, the result shows unrealistic posterior emission estimates, indicating an issue from the inversion setup to be resolved before proceeding to the originally planned 1 year long CH_4 inversion estimates. Nevertheless, we have identified several shortcomings and are working on potential solutions to overcome them.

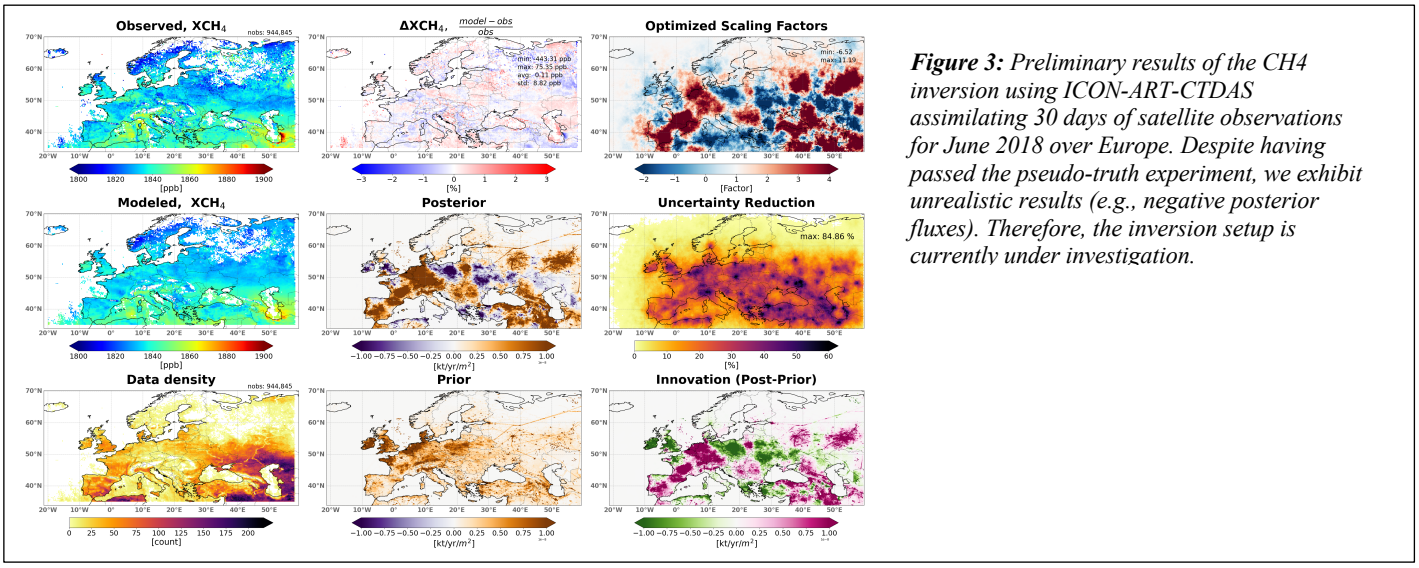

Figure 3: *Preliminary results of the CH4 inversion using ICON-ART-CTDAS assimilating 30 days of satellite observations for June 2018 over Europe. Despite having passed the pseudo-truth experiment, we exhibit unrealistic results (e.g., negative posterior fluxes). Therefore, the inversion setup is currently under investigation.*

-WRF-CHEM (1km resolution): Using the resources of bm1400, we have done analyses on the difference between the Building Effect Parametrization (BEP) and Urban Canopy Model (UCM) in WRF to optimize the use for urban analysis. We have found that UCM outperforms BEP in the current settings with respect to temperature, wind speed, and wind direction at urban sites.

Module Q&S:

-LandscapeDNDC: The model framework has been successfully tested at relatively low spatial (25 x 25 km) and temporal (yearly outputs) resolution based on the simulation of a representative sub-sample (N=50.000, ~50 sites per grid cell) out of a total of approximately 10 million agricultural fields of Germany. The model's internal clock always runs hourly, but the output is currently aggregated into yearly sums for comparison with the national inventory reporting. First comparisons to the national GHG inventories (NIR) show a good match (Figure 4). The LandscapeDNDC framework was also transferred to forest ecosystems after its successful application on agricultural soils. With a time delay of approximately half a year, we are currently testing it at relatively low spatial (25 x 25 km) and temporal (yearly outputs) resolution. It can be envisaged that for the last quarter of 2024 or the first quarter of 2025, we will reduce the temporal and spatial resolution, leading to a further increase in computational and storage demands.

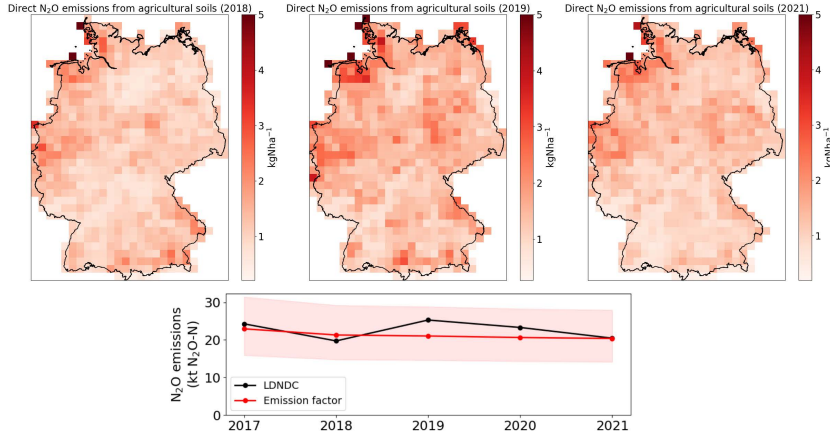

Figure 4: *LandscapeDNDC estimates of N_2O emissions from agricultural land at a yearly timescale for 2017 - 2021 (black line). This is compared to the National GHG inventory reporting (red line and shaded red error estimate). The simulated emissions are well within the error margin of the NIR but are able to better capture the influence of climatic conditions (dry year in 2018 vs. high yields in 2019).*

Additional benefits from Swift Object Storage: Swift Object storage space have so far been used for the submission of deliverables generated for work packages within the modules (e.g. model output from LandscapeDNDC for use by Module M). Most Module Q&S projects granted in 2024 started with providing low-resolution datasets to the ITMS system (transition from 25 x 25 km to 5 x 5 km and below), exemplary datasets, or datasets with yearly aggregations. With the continuation of ITMS in 2025 and beyond, it is envisaged that the temporal and spatial resolution will increase significantly, leading to increased data space consumption.

Justification for under-utilization of the allocated resources in 2024:

We acknowledge a low utilization of allocated resources for the period of January to October 2024, most of which is related to a delayed start of the multiple groups involved. Several groups have joined with a delay and just started implementing their simulations on Levante. At this early phase in the project, also many novel experiments have started, that need initial testing at smaller scales to assess their benefit before scaling up to a full simulation. The reasons for the low utilization within the different Models and simulations are listed here:

1. CSR + STILT (0.25 x 0.25 degrees)/ ICON-ART - CTDAS (R3B08, 6.5 km resolution): At the MPI-BGC, there has been an incomplete transfer of computational work from our mj0143 project to the bm1400 project and this is ongoing. Furthermore, the Rn and the CH_4-Rn dual-tracer inversions have so far only covered a single year due to testing and development of the dual-tracer approach.
2. ICON-ART simulations (R2B06, 40 km resolution): Although scaling tests were carried out, during the 2024 allocation period we focused mostly on developing a new super-simplified OH chemistry and corresponding model setup due to some recent shifts in priorities within the project. However, we plan to start ICON-ART simulations within the remaining 2024 allocation period. The development of the new model setup is close to being finished and in 2025 we will proceed with the long and computationally heavy simulations requested for 2025.
3. Pre- and Post-processing using CDO, NCO, and Python, Statistical assessment and fitting of mathematical models with Python, Dask, and CDO: So far, we have been directly working at the RCL supercomputer and began the adaptation of the ITMS-M-DWD pre-operational system at the ECMWF supercomputer in Bologna. The reasons are; (a) the ease of accessing the meteorological, emission (RCL), and atmospheric composition (Bologna) datasets for creating the emission datasets, and the initial and boundary conditions; and (b) that the NWP simulations and the data assimilation and inversion are and will continually be performed at those platforms. Therefore, the pre-processing and some diagnostic tools have been tested at Bologna and used in-production at RCL, instead of implementing them at Levante. Given that the first results of our system demonstrator came out just some months ago, the planning and execution of data sharing is already beginning from our side, hence why we have requested the same amount of Levante and Archive storage as in 2024 but a reduced computing time.
4. LandscapeDNDC: The focus during 2024 has been setting up a model framework and small-scale testing. This was performed on the local HPC cluster at IMK-IFU and the cluster in Karlsruhe, since these computers already had the model code and libraries running, and data ingestion frameworks were already established. This phase is now almost complete and we are about to transfer the setup to Levante. Thus, from early 2025, we can start performing more computationally intensive model runs. We will additionally profit from the regionalized meteorological data available on Levante.
5. FLUXCOM-X: We are currently behind schedule in utilizing the allocated resources. The Q&S_II project TORCH, granted in 2024, began slightly later than planned with the onboarding of a new team member in the summer. After they became familiar with the code base and programming environment, we compiled and preprocessed essential site-level and satellite-based input data on Levante. With these preliminary steps now complete, we plan to begin utilizing the allocated resources towards the end of the year 2024 to generate a flux ensemble.
6. Additional Swift Object Storage: Due to the delayed start of some of our project partners, we have so far used less than 2% of the total granted capacity for 2024. However, increased usage as a data management and documentation platform is foreseen in the upcoming allocation phases along with the direct use of Levante by Module M.