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DKRZ Computing Resources Report - 2026/01 - 2026/10

Principal Investigator	Prof. Jia Chen, Technical University of Munich
Project Name	Advances in Urban GHG Emission Modeling
Reporting Period	01.01.2026 – 31.10.2026

1 · Resource Usage

In the period 2026-01-01 to 2026-12-31 we were granted 18,259 CPU node hours, 2,480 GPU node hours and 25 TB of Levante storage. As of October 31, 2026, we have used ~ 72 % of the CPU node hours and ~110 % of the GPU node hours allocated for the year of 2026 (excl. expired node hours). We were able to move more experiments than expected to GPU-accelerated simulations, and plan to use the remaining 28 % of allocated CPU node hours by the end of the year – if scheduling permits it. Due to the high computational demand of our PALM4U simulations and the cut in requested resources, we've decided to permanently move the PALM4U simulations to a different compute cluster and will not request resources for this again in the 2027 allocation period.

2 · Scientific Progress

WP1 · Ultra-High-Resolution Transport Using GRAMM/GRAL and Biogenic Flux Modeling led by Junwei Li

Building on our established and validated framework for CFD-based CO_2 dispersion modeling in Munich, we further refined the workflows and incorporated updated input datasets to extend and improve our simulations. Hourly CO_2 concentration fields were simulated at 10 m resolution for Munich over the period 2019–2025.

Based on this ultra-high-resolution transport model, we developed and iteratively refined an inversion framework combining Markov Chain Monte Carlo (MCMC) sampling with Gaussian Processes (GPs) to constrain the spatial and temporal distribution of urban CO_2 emissions, a method critically dependent on the GPU acceleration provided by Levante. A range of observing system simulation experiments (OSSEs) was conducted to evaluate the framework. The resulting framework was applied to Munich for 2024 and 2025, combining simulated hourly CO_2 concentration fields with observations from the mid- and low-cost sensor networks to assess CO_2 emissions.

In support of this inversion and WP4, we generated hourly biogenic CO_2 flux inventories at the same resolution over the same seven-year period. We published our high-resolution biogenic flux modeling in Earth's Future.

WP2 · GHG Transport Modeling With WRF-CTDAS and Footprint Modeling led by Haoyue Tang

We conducted a sensitivity analysis of WRF at 1 km resolution, testing different data assimilation strategies across multiple physics configurations to assess their effects on meteorological fields and downstream LPDM (Lagrangian Particle Dispersion Model) simulations. Through this investigation, we provided a comprehensive assessment of the influence of model configuration on greenhouse gas inversion results.

Based on this assessment, we ran WRF using the RETRO footprint modeling framework for 2023–2025, generating meteorological fields and footprints to support the evaluation of atmospheric transport accuracy and the inverse modeling studies conducted in WP4. These simulations provided an additional meteorological driver for these applications. We also began using the resulting footprints in CTDAS experiments to optimize greenhouse gas fluxes.

WP3 · Footprint Modeling led by Moritz Oliveira Makowski

We continued improving our footprint modeling framework RETRO (REgional TRansport Operators) using the DKRZ HPC infrastructure. RETRO introduces a significant accuracy improvement in how LPDM-based footprints are calculated by using local turbulence information to compute the sensitivity of different atmospheric layers to surface fluxes. This improvement has been validated by conducting extensive forward-backward simulations on Levante, i.e., by running HYSPLIT forward and backward in time and evaluating the mismatch for ERA5 and HRRR meteorology, demonstrating universal applicability of the RETRO framework.

Secondly, due to the GPU capability of ICON, running ICON over long periods of time is much more affordable than running WRF over long periods of time. Hence, we've set up an ICON-LAM (ICON in Limited Area Mode)

environment on our local workstations and conducted the footprint runs for all of these new meteorological fields on Levante. Using our own wind LiDAR observations, we could show a significant improvement in ICON-based footprints compared to ERA5-based footprints, with strong agreement between ICON and WRF footprints.

As planned, we also continued our investigation of using ultra-high-resolution meteorological fields produced by GRAMM/GRAL or PALM4U in the footprint modeling stage. Our preliminary conclusion on this is that the first major gain in footprint accuracy is obtained when resolving the terrain correctly, and the second major gain is only obtained when resolving the building structure correctly. This second gain only occurs at horizontal resolutions of less than 5 m, which is too expensive to run for long periods of time due to memory consumption.

WP4 · Inverse Modeling led by Josef Stauber and Tobias Grasberger

The biogenic flux estimates resulting from WP1, as well as the WRF, ERA5, and ICON footprints generated in WP2 and WP3, are essential for the inverse modeling studies conducted by Josef Stauber and Tobias Grasberger.

The data generated in 2026 and previous allocation periods were used to assess Munich's CO_2 emissions from 2020 to 2025 using Bayesian inversion with ground-based total column observations generated by MUCCnet. The emission reduction based on the observations was compared with the estimation from the city of Munich. This work is currently in review for IEEE Transactions on Geoscience & Remote Sensing. We also integrated our in-situ observations from Munich into this inverse modeling framework, but noticed model-data mismatches so large that the transport model errors need to be addressed first (as done in WP3 in this allocation period).

Different methods for adapting Compressed Sensing (CS) to the atmospheric inversion workflow have been investigated and tested, with the aim of recovering urban greenhouse gas emission fields by focusing on their main drivers. This work is currently in review for the EGU journal Geoscientific Model Development, and showcases the ability of our approach on synthetic data to be able to separate sparse point sources and smoothed wide-area sources in an urban emission field. We also successfully applied CS to recover and pinpoint real SF_6 point sources over Europe.