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DKRZ Computing Resources Report - 2025/01 - 2025/10

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Project Name	Advances in Urban GHG Emission Modeling
Reporting Period	01.01.2025 – 31.10.2025

1 · Resource Usage

Out of the requested 32,250 CPU node hours and 51 TB of Levante storage, we were granted 9,998 CPU node hours and 29 TB of Levante storage for the allocation period from 2025/01 to 2025/12, which is the average cut for community projects in 2025. As of October 30, 2025, we have used approximately 13,000 CPU node hours and 2,200 GPU node hours due to being able to run computations on weekends when the cluster is not fully occupied. Due to the cut in resources, we decided to run our OpenFOAM simulations on a different compute cluster.

2 · Scientific Progress

High-Resolution Modeling Using WRF and WRF-GHG/WRF-Chem — led by Haoyue Tang

We ran WRF-Chem for 2023 and part of 2025, providing meteorological fields and CO_2 and CH_4 simulations over Europe. We observed significant issues in vertical mixing, likely related to the choice of urban physics and PBL dynamics schemes. This required more careful investigation before running the model for other years.

In parallel to using WRF as a source of high-resolution meteorological fields for our inverse modeling frameworks, we started to use WRF-CTDAS, which assimilates GHG observations into WRF-Chem simulations. WRF-CTDAS uses an Ensemble Kalman filter (EnKF) approach to optimize surface emission and background concentration.

Ultra-High Resolution Biogenic Flux and CFD Modeling Using VPRM and GRAMM/GRAL — led by Junwei Li

To accurately quantify anthropogenic GHG emissions in urban areas, we need to quantify biogenic fluxes in urban areas as well. Given the absence of a high-resolution biogenic CO_2 flux inventory, we used the Vegetation Photosynthesis and Respiration Model (VPRM) with Sentinel-2 data to create an ultra-high-resolution (10 m) biogenic CO_2 flux inventory. This inventory was used to drive the GRAMM-SCI/GRAL-ST-ROG CFD model, generating ultra-high-resolution (10 m) meteorological fields as well as hourly CO_2 concentration fields.

Inverse Modeling Using GRAMM/GRAL — led by Junwei Li

By running GRAMM/GRAL in a way that stores the relationship between surface fluxes and atmospheric concentrations, we could perform an inverse correction of the a priori anthropogenic CO_2 emission inventory. This was done by assimilating data from our CO_2 observation networks into these forward simulations. This inversion method employed a Gaussian Process model, a method critically dependent on the GPU acceleration provided by Levante.

Ultra-High Resolution CFD Modeling Using PALM-4U — led by Vigneshkumar Balamurugan

The high-resolution LES model PALM-4U has been set up for the Munich domain to simulate air pollutant dispersion within urban areas at high spatial (up to 10 m) and temporal resolutions (10 minutes). We incorporated different chemistry mechanisms with varying computational demands have been incorporated into the PALM-4U model and compared against observations to study the complexity of secondary pollutant formation. Fortunately, the cut in computing resources coincided with a blocking issue in the model. Since the bug has been fixed by now, we can continue this investigation in 2026.

Footprint Modeling Using HYSPLIT and STILT — led by Moritz Makowski

The meteorological fields generated by ERA5 and WRF were used to drive the Lagrangian Particle Dispersion Model (LPDM) HYSPLIT in order to generate STILT footprints used in the inverse modeling frameworks mentioned below. Significant effort went into making the generation of these footprints more efficient and reliable. We implemented an updated STILT methodology and conducted a comparison with controlled release experiments conducted by NOAA to validate our improvements. Significant effort was made to use 10 m resolution CFD wind fields to compute surface flux footprints. We are now able to generate these footprints based on ultra-high-resolution wind fields and plan to compute them for a long time period in 2026 to be used in our inverse modeling frameworks. In addition to surface fluxes, we examined the variability of the air entering our modeling domain. We connected our observations to nudged CAMS and ICON-ART simulations to reduce the uncertainty in background concentrations.

Inverse Modeling Using Bayesian Inversion led by Josef Stauber

We aim to estimate the total CO_2 emissions of Munich using MUCCnet (total column measurements). To link the measured CO_2 concentrations to emission fluxes, accurate transport models are required. Uncertainty in the transport process outweighs measurement uncertainty, so improving transport models reduces posterior uncertainty most effectively. Using Bayesian inversion enables us to solve the equations analytically and produce a trend of Munich's CO_2 emissions since 2019. This trend is then compared to those from the emission inventories to verify the path towards climate neutrality of Munich by 2035. In 2026, we will integrate in-situ CO_2 observations from our Mid-Cost sensor network. For this effort, there is an even greater need for accurate transport models given that the network is situated on rooftops within the complex urban terrain.

Inverse Modeling Using Compressed Sensing led by Tobias Grasberger

In the our sparse inversion framework, we solve the Basis Pursuit Denoising problem to reconstruct the original high-dimensional emission field using observations and footprints, while applying a regularization technique that enforces sparsity in the solution. The algorithm primarily enables the recovery of point sources. A variation of this framework allows for the inclusion of a compressive encoding of the emission field, which only captures the main driving forces behind urban emissions. This variation reduces the number of required observations for a given inversion performance.

3 · Publications

Journal publications on each of the points mentioned above are in preparation. The work done on these items has already been presented at the following conference talks:

[1] J. Stauber, J. Chen, F. Klappenbach, J. Li, A. Luther, M. Makowski, H. Tang, N. Ponomarev, D. Brunner, Assessment of Munich's CO2 emissions via Bayesian inversion using MUCCnet data from 2020-2025, (2025). https://doi.org/10.5194/egusphere-egu25-17841

[2] V. Balamurugan, J. Chen, H. Saathoff, C. Claus Holst, A. Wenzel, A. Abu-Hani, Y. Li, Y. Li, S. Abou-Rizk, F. N Keutsch, High-Resolution LES-Based Air Quality Modeling Over Munich: Evaluation of Model Performance, and Pollution Drivers, (2025). https://doi.org/10.5194/egusphere-egu25-16731

[3] J. Chen, J. Stauber, J. Li, P. Aigner, D. Kühbacher, M. Makowski, A. Luther, A. Wenzel, H. Tang, J. Hinderer, F. Dietrich, C. Asam, Observational and Modeling Tools for Monitoring Urban Greenhouse Gas Emissions: Results of the ICOS Pilot City Munich, (2025). https://doi.org/10.5194/icuc12-721