Project: **1233**

Project title: **MOD: DataWave**

Principal investigator: **Claudia Stephan**

Report period: **2025-11-01 to 2026-10-31**

Maximum of 15 pages including figures. 9 pt minimum font size.

Project overview

MOD: DataWave is an umbrella DKRZ project supporting five externally funded research projects conducted within the Modelling of Atmospheric Processes (MOD) department at the Leibniz Institute of Atmospheric Physics (IAP). Our department develops and applies UA-ICON, the upper-atmosphere extension of the ICON atmospheric modelling system. The five projects address complementary scientific questions and/or model development priorities.

DataWave (funded by Schmidt Sciences; 1 postdoctoral researcher)

The influence of the lower atmosphere, including the troposphere and stratosphere, on the upper atmosphere—the mesosphere, thermosphere, and ionosphere—is an increasingly active area of solar-terrestrial physics. The multiscale dynamics of these upper-atmospheric regions are strongly influenced by atmospheric tides, gravity waves, and small-scale turbulent eddies. Using UA-ICON, we investigate the life cycles of explicitly resolved waves, tracing their propagation from source regions to dissipation and examining their interactions with other waves, the mean flow, and turbulence. UA-ICON simulations provide insight into the mechanisms governing energy transfer across atmospheric scales.

IMPAGT (funded by the Leibniz Association; 1 postdoctoral researcher, 2 PhD students)

IMPAGT stands for *Investigating MLT Processes with Atmospheric Modelling from Ground to Lower Thermosphere*. Funded through the Leibniz Best Minds Programme for Women Professors, the project focuses on the development of UA-ICON to improve the representation and understanding of processes in the mesosphere and lower thermosphere (MLT). Launched in 2024, IMPAGT is a long-term model development effort that will continue over the coming years. Its activities contribute directly to advancing the model capabilities shared across the department.

TRR181 (funded by the DFG; 1 postdoctoral researcher, 1 PhD student)

TRR181 is the Collaborative Research Centre *Energy Transfers in Atmosphere and Ocean*. MOD contributes to two work packages (W6 and S2), focusing on energy transfer across scales and the representation of turbulence in atmospheric models. Although wave energy spectra exhibit robust spectral slopes, the physical mechanisms responsible for these patterns remain incompletely understood. Using UA-ICON, we investigate spectral energy transfer in both global and regional domains, linking the inferred transfer processes to different meteorological regimes and enabling validation against observations. In parallel, we are implementing an improved turbulence closure scheme in ICON based on the dynamic Smagorinsky approach.

Keystone (funded by the European Space Agency, ESA; 1 postdoctoral researcher)

Keystone is a candidate ESA Earth Explorer 12 mission designed to investigate the mesosphere–thermosphere system and its role in connecting Earth's atmosphere with near-Earth space. In 2024, I was selected to serve on the Mission Advisory Group. Since 2025, I have contributed to the Science and Requirements Consolidation (SciReC) study and to the design of an end-to-end performance simulator led by industry. UA-ICON simulations are used to characterize atmospheric variability and assess how it would be observed by the proposed Keystone instruments, linking atmospheric processes, instrument performance, and the mission's scientific objectives.

AIR-MoPSy (funded by the European Union; 1 postdoctoral researcher)

Global Navigation Satellite Systems (GNSS) provide essential positioning and time-synchronization services. Natural disturbances and human-induced interference can disrupt GNSS signals, potentially compromising safety-critical air and maritime traffic. AIR-MoPSy aims to develop R-Mode as a resilient backup navigation system capable of providing sufficiently accurate positioning and timing during GNSS outages. Our contribution focuses on UA-ICON simulations to investigate atmospheric influences on the D-layer of the ionosphere, whose state and variability are important for the accuracy and reliability of R-Mode navigation.

Report

This report is organized into seven sections. Section 1 summarizes the most significant developments in the UA-ICON code since the previous report. Sections 2–6 present selected highlights from the five projects described above. Section 7 summarizes the most relevant additional uses of the computational resources allocated to this project.

1. Summary of Code Evolution

1.1. Code Governance

UA-ICON extends ICON with a deep-atmosphere dynamical core and additional parameterizations of upper-atmospheric physical processes, including molecular diffusion, ion drag and Joule heating, frictional heating, radiation, and interactive chemistry.

To ensure the long-term sustainability of MOD's model developments, we have restructured the ICON source code, moving as much UA-specific functionality as possible into a dedicated directory, icon-nwp/src/upatmo. This restructuring was agreed upon jointly with DWD, DKRZ, and MPIM. The German Weather Service (DWD) has since transferred full responsibility for changes within this directory, whether made by MOD or other contributors, to our department. This arrangement is supported by automated bot notifications, helping to ensure transparent coordination and clear responsibility for code maintenance.

1.2. Extension of the Model Domain

Building on a MSc project investigating numerical stability in the thermosphere, we have successfully extended the upper boundary of UA-ICON to an altitude of 400 km.

1.3. Physics-Related Code Developments

- **New parameterization of thermospheric viscosity** (MSc thesis)

  We are developing an energetically consistent implementation of the physical parameterizations used in UA-ICON. The individual components are being systematically evaluated, with particular emphasis on their effects on numerical stability and the consistency of energy transfer between physical processes.

- **Interactive chemistry and short-term solar variability** (DFG project SODYMLT)

  Developments in interactive chemistry and the representation of short-term solar variability are covered by a separate compute time proposal (Project: 1435, Solar activity and dynamics of the mesosphere and lower thermosphere).

- **ML parameterization of ion drag and Joule heating** (IMPAGT PhD project)

  The machine-learning model has been trained and validated, and a manuscript describing the results has been prepared for submission. We are now integrating the model into ICON using FTorch. This work is progressing well, supported by the expertise of our scientific programmers, who are also developers of FTorch.

- **Dynamic Smagorinsky turbulence scheme** (TRR181 postdoctoral project)

  The Dynamic Smagorinsky Model (DSM) was previously adapted for the spectral atmospheric model KMCM. Implementing it in ICON presented a substantial technical

challenge: the filtering procedure used in the spectral model had to be adapted to ICON's unstructured triangular grid. We addressed this challenge by developing a coarse-graining-based filtering approach suitable for the ICON grid. We then implemented the diagnostic formulation used to determine the Smagorinsky coefficient dynamically and coupled the resulting coefficient to the horizontal diffusion scheme of the ICON dynamical core. This allows the turbulence parameterization to respond consistently to the resolved flow. A three-month simulation has been completed to assess the numerical stability of the implementation. Based on these results, we are preparing a manuscript for submission this year.

- **Composition-dependent thermodynamics** (Keystone postdoctoral project)

  UA-ICON has so far treated atmospheric air as a well-mixed dry gas. This assumption leads to substantial underestimation of the atmospheric scale height in the upper atmosphere: approximately 20% at 150 km and a factor of two or more at altitudes of 400–500 km.

  Our analysis of the model equations has shown that, given ICON's prognostic variables—density and Exner pressure—the effects of variable atmospheric composition can be incorporated through a small number of identifiable terms, without changing the momentum equations or the equation of state. One of these terms, previously applied only to water vapor, determines the adiabatic heating of an atmosphere dominated by atomic oxygen. These findings indicate that ICON's existing prognostic framework can support a variable-composition thermosphere while maintaining mass and energy conservation. This provides a promising route towards a more physically consistent representation of thermospheric structure and dynamics.

1.4. Data Assimilation

Another important development is the introduction of data assimilation capabilities through the Data Assimilation Research Testbed (DART). To enable DART to work with ICON, we have developed an interface for reading and writing ICON restart files. We have also implemented software to obtain operational meteorological products and satellite observations of the upper atmosphere. An initial two-month test of the resulting data assimilation system is currently underway. This test will provide a first assessment of the integrated workflow and its suitability for future UA-ICON applications.

1.5. Operational Applications of UA-ICON

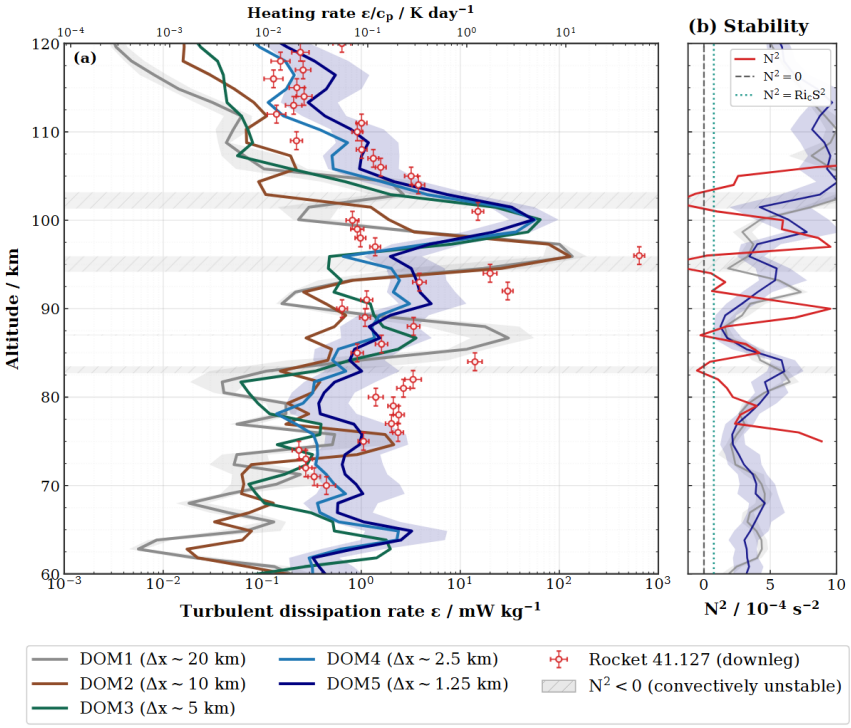
UA-ICON has matured into a high-quality whole-atmosphere modelling system and is now being prepared for operational forecasting applications. The model has recently been ported to the Deutsches Meteorologisches Rechenzentrum (DMRZ), where the Bundeswehr Space Command (Weltraumkommando der Bundeswehr) will conduct its first operational forecasts in collaboration with MOD. This marks an important step towards transferring UA-ICON from research and development into operational use.

2. DataWave

2.1. Rocket campaign

Publication (resubmitted): Y. A. Morfa, M. Kunze, T.A. Siddiqui, C. Zülicke, C.C. Stephan, G. Lehmacher, M. Mossad, R. Wing, I. Strelnikova, G. Baumgarten, T. Renkwitz, J.M. Urco, R. Latteck, J.L. Chau, and C. Stolle: “Whole-atmosphere modeling with regional refinement: Strengths and drawbacks assessed with observations from the VortEx campaign”, *Journal of Advances in Modeling Earth Systems*

This resubmitted paper now contains a sophisticated comparison of rocket data to UA-ICON:



(Left) Measured turbulent dissipation rates and parameterized subgrid-scale dissipation across all five domains. Shaded bands indicate the interdecile range within the sampling volumes of DOM1 and DOM5. (Right) Squared buoyancy frequency measured by the rocket, compared with the median values from DOM1 and DOM5.

2.2. Seismoacoustic analysis

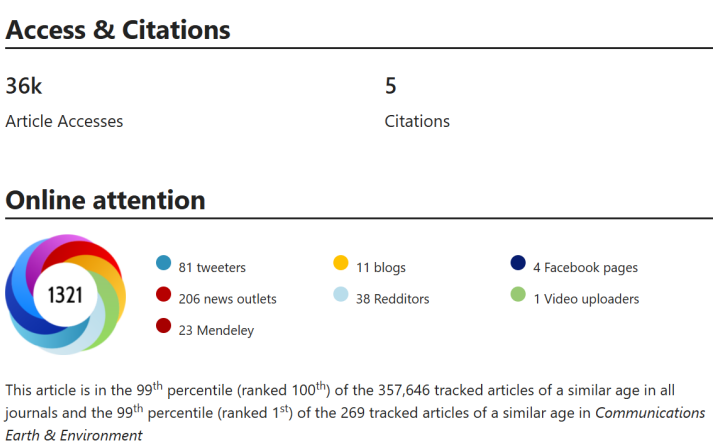
Publication (published): Hupe, P., Pilger, C., Assink, J. et al. Seismoacoustic Analysis of a Falcon 9 Rocket Stage Re-Entry Over Central Europe on 19 February 2025. Pure Appl. Geophys. (2026). https://doi.org/10.1007/s00024-026-04106-9

MOD contributed its atmospheric modelling expertise to the study by analysing atmospheric conditions affecting infrasound propagation during the re-entry of a SpaceX Falcon 9 rocket stage. This contribution supported the interpretation and validation of observed seismoacoustic signals, helping to elucidate how small-scale atmospheric dynamics influence signal propagation and the detection of re-entering space debris.

2.3. Lithium plume

Publication (published): R. Wing, M. Gerding, J. Plane, Y. Morfa, J. Urco, Y. Yamazaki, L. Schulz, J. Höffner, J. Mielich, T. Renkwitz, C.C. Stephan, G. Baumgarten, C. Stolle (2026): “Measurement of a lithium plume from the uncontrolled re-entry of a Falcon 9 rocket”, *Nature Communications Earth & Environment*, 7 (161) doi: 10.1038/s43247-025-03154-8

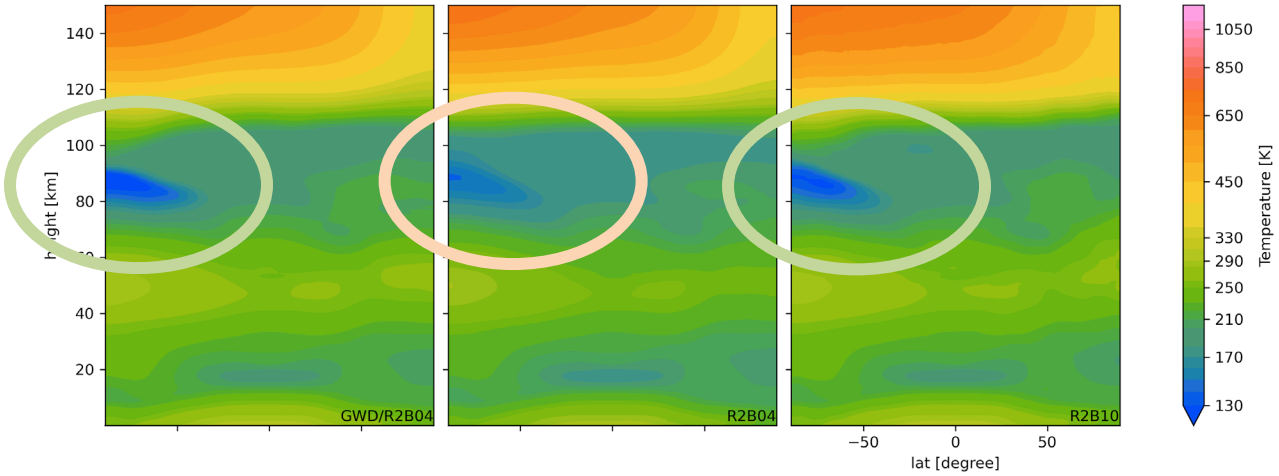
Using UA-ICON simulations and back-trajectory calculations, MOD helped reconstruct the atmospheric transport of the lithium plume and trace its origin to the uncontrolled re-entry of the Falcon 9 rocket stage. By combining model results with lidar and meteor radar observations, the study characterized the atmospheric conditions governing plume transport and strengthened the attribution of the observed lithium enhancement to the rocket re-entry.



This paper has received tremendous attention (as of 22.10.26).

3. IMPAGT

3.1. The convergence experiment



We conducted a series of global simulations, starting from our tuned R2B4 configuration (approximately 160 km grid spacing) with the gravity wave parameterization enabled (left panel). We then switched off the parameterization (middle panel) and progressively increased the horizontal resolution, reaching R2B10 (approximately 2.5 km grid spacing) in the highest-resolution simulation (right panel).

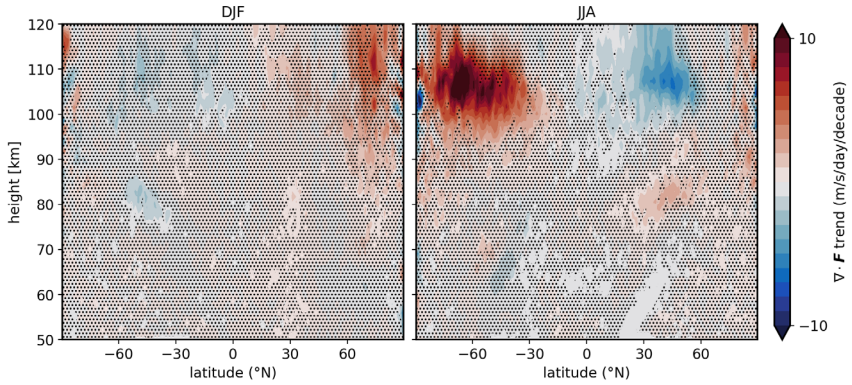
The objective is to determine at what resolution an explicit representation of atmospheric dynamics becomes sufficient to reproduce the observed overturning circulations in the mesosphere and thermosphere without the need for a gravity wave parameterization. Preliminary results indicate convergence towards a consistent solution as the resolution increases. Beyond their scientific value, these simulations represent a substantial technical achievement, demonstrating our ability to conduct global UA-ICON simulations at kilometre-scale resolution. A publication based on this work is in preparation (IMPAGT postdoctoral project).

3.2. The climate change experiment

Anthropogenic carbon dioxide (CO_2) emissions are widely recognized as the primary driver of global warming. Beyond their warming effect at Earth's surface, increased CO_2 concentrations enhance radiative cooling and contribute to the contraction of the middle atmosphere. These thermal changes, together with changes in the large-scale circulation of the troposphere and stratosphere, also influence long-term trends in the mesosphere and lower thermosphere (MLT).

Gravity waves play a fundamental role in driving MLT dynamics and shaping its thermal structure. We therefore selected a horizontal grid spacing of 20 km to explicitly resolve a substantial portion of the gravity wave spectrum. To maintain a realistic representation of the large-scale atmospheric circulation up to an altitude of 50 km, the tropospheric and stratospheric dynamics are constrained by the ERA5 reanalysis dataset from ECMWF.

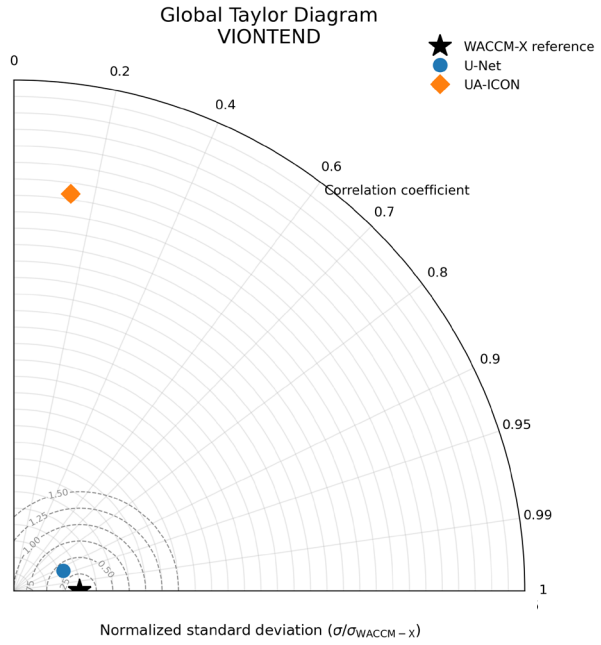
Temperature fields from the simulations are used to characterize the climate change signal in the MLT region. In addition, we apply the Transformed Eulerian Mean (TEM) framework to investigate long-term trends in gravity wave activity and wave–mean flow interactions. The model results are evaluated against the JAWARA dataset, a whole-neutral-atmosphere reanalysis generated using the Japanese Atmospheric General Circulation Model for the Upper Atmosphere Research–Data Assimilation System (JAGUAR-DAS). IMPAGT PhD1 is preparing a publication presenting the trend analysis.



Linear trend in gravity-wave-related Eliassen–Palm (EP) flux divergence. Hatched regions indicate trends that are not statistically significant at the 95% confidence level. Significant trends are evident in the lower thermosphere, with emerging signals also apparent in the mesosphere.

3.3. Geomagnetic storms in UA-ICON

Ion drag and Joule heating are key processes governing momentum and energy transfer between the ionosphere and thermosphere, but their computation remains costly in whole-atmosphere models. This study explores deep learning as a computationally efficient surrogate for these processes using simulations from WACCM-X. A convolutional U-Net is developed to predict Joule heating and ion-drag-induced zonal and meridional neutral-wind tendencies from atmospheric and geophysical inputs. The model incorporates spatial, temporal, vertical, and external forcing features, with different loss functions tested to better capture localized auroral activity. Evaluation on independent validation periods shows that the model reproduces the main spatial and temporal patterns of ion drag and Joule heating, highlighting its potential for efficient integration into atmospheric simulations. IMPAGT PhD2 has finished a draft of her first paper.



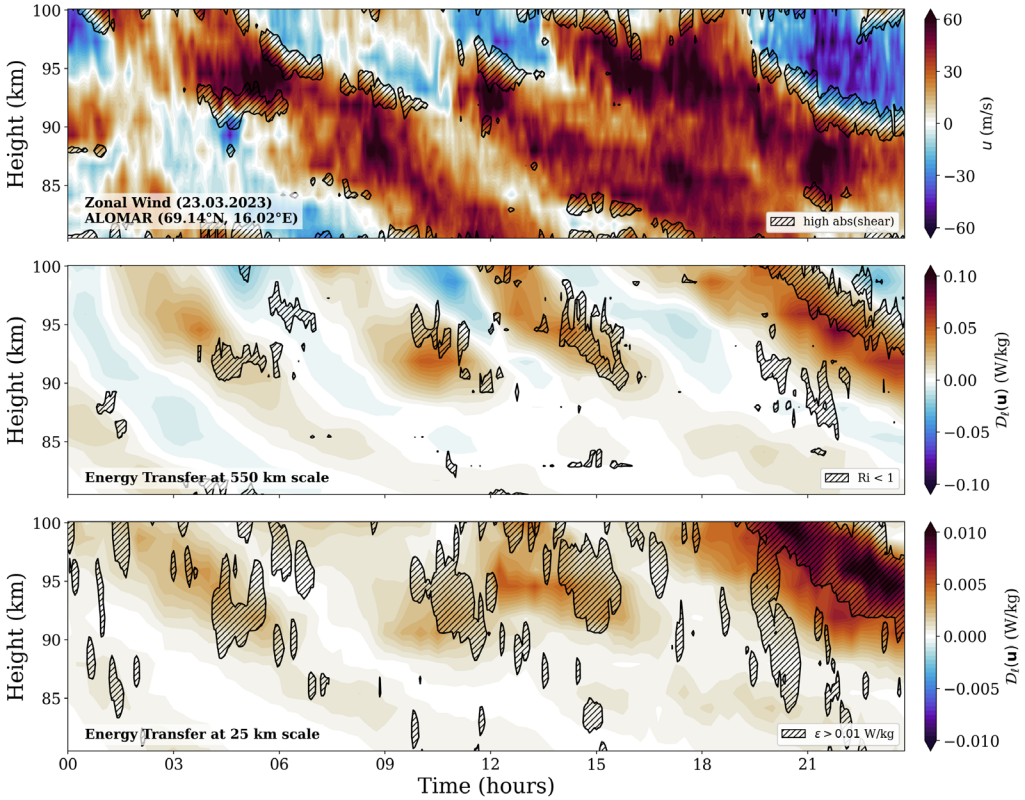
The meridional wind tendency due to ion drag in the master branch of ICON (UA-ICON) and in our newly developed version (U-Net).

4. TRR181

4.1. Regional spectral energy transfer

Resolving ongoing debates between competing theories of energy transfer across horizontal scales requires diagnostic methods that go beyond traditional spectral analyses. We address this challenge by combining local physical-space diagnostics with high-resolution, nonhydrostatic spectral energy budgets in regional domains. Our approach provides three-dimensional maps of instantaneous energy transfer at specific scales, enabling us to identify the atmospheric structures responsible for these transfers, including breaking waves. This offers a complementary perspective to conventional diagnostics based on global or domain-averaged spectra. In parallel, we employ a moist, nonhydrostatic spectral energy budget that quantitatively partitions energy redistribution into nonlinear transfers, vertical flux divergences, and buoyancy conversions. Together, these complementary approaches reveal where energy transfers occur in physical space and how energy is redistributed across scales. We first applied these combined

methodologies to idealized UA-ICON simulations of mountain waves and subsequently extended the analysis to realistic UA-ICON simulations. Our TRR181 PhD student is currently preparing his first manuscript on energy transfers in spectral and physical space.



Top: Tides as seen in the zonal wind (contours) induce shear (shaded area). Middle: Mesoscale energy transfers, here across a horizontal scale of 550 km, are related to shear produced turbulence (shaded area). Bottom: Energy transfers at near grid scale (R2B7 grid), here across a horizontal scale of 25 km, align with high dissipation rate as parametrized by ICON (shaded).

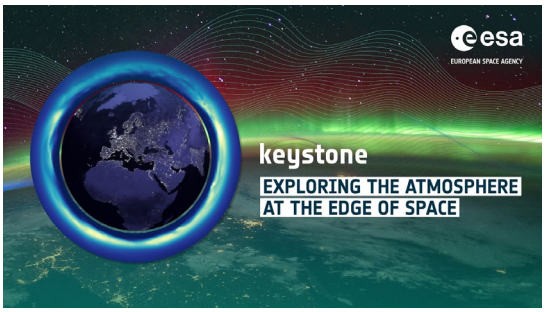
4.2. Turbulence closure

The TRR181 postdoc has implemented the Dynamic Smagorinsky closure and is also preparing a publication (see section 1.3).

5. Keystone

Keystone is a candidate for the European Space Agency's (ESA) twelfth Earth Explorer mission (EE12), designed to investigate the mesosphere–thermosphere system and its role in connecting Earth's atmosphere with near-Earth space. The mission aims to improve our understanding of upper-atmospheric composition, dynamics, and energy balance through satellite observations of atmospheric constituents, temperature, and winds. The Leibniz Institute of Atmospheric Physics (IAP) contributes to the mission's scientific preparation through its involvement in the Mission Advisory Group and the Science and Requirements Consolidation (SciReC) study. A key contribution from the MOD department is the use of UA-ICON, to characterize atmospheric variability and assess the expected scientific performance of different satellite orbit and instrument-viewing configurations. Global UA-ICON simulations are used to generate synthetic Keystone observations, allowing us to evaluate how effectively the proposed instruments could capture atmospheric wind structures and variability. These results support the refinement of mission requirements and the design of the end-to-end performance simulator in collaboration with industrial partners.

The SciReC team is also preparing a journal publication. In addition, a MSc student has recently started her thesis in the MOD department, continuing the analysis of synthetic Keystone observations generated from UA-ICON simulations.



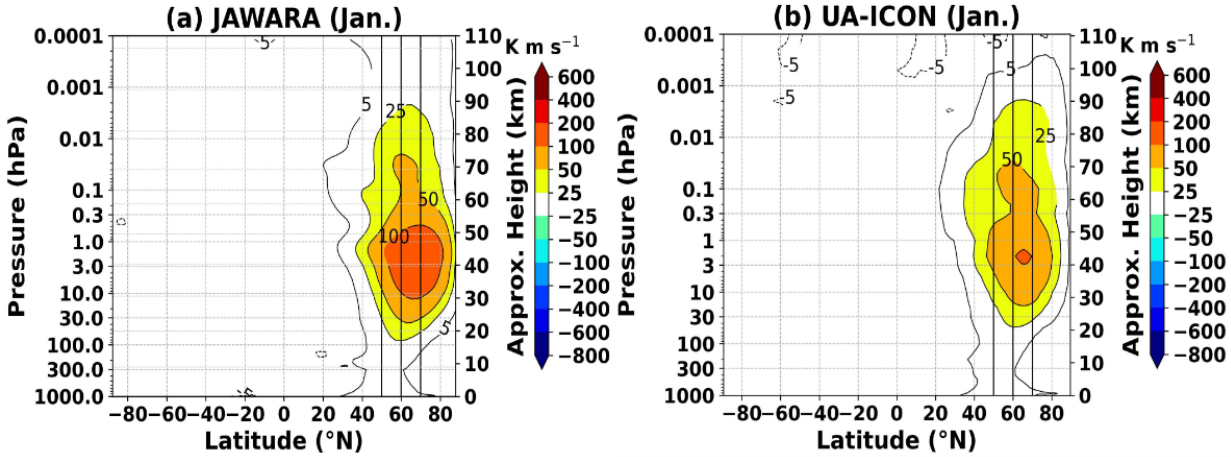


DKRZ receive acknowledgement in our Keystone presentation shown at the 2026 user consulation meeting.

6. AIR-MoPSy

Publication (under review): P. Ghosh, D.W. Peters, C.C. Stephan: "Quasi-Stationary Wave-Driven Circulation over the Baltic Sea Region - A Comparison Between JAWARA Reanalysis and UA-ICON", *JGR-Atmospheres*

The performance of the UA-ICON general circulation model in representing large-scale atmospheric dynamics over the Baltic Sea Region (BSR; 50°–70° N, 10°–30° E) is evaluated against the JAWARA reanalysis (2005–2024). The analysis focuses on seasonal variations in horizontal winds, geopotential height, temperature, and quasi-stationary wave (QSW) propagation. UA-ICON captures the seasonal cycle of strong wintertime westerlies, peaking near 50 km, but underestimates QSW amplitudes near 1 hPa and exhibits an eastward phase shift of approximately 30° relative to JAWARA. Differences are more pronounced in the mesosphere–lower thermosphere (MLT), where UA-ICON simulates weaker meridional wind structures. It also underestimates the enhanced interannual variability of stratopause zonal winds over the northern BSR, reproducing this feature primarily in the south. Despite these discrepancies, QSW heat fluxes show good local agreement in the middle atmosphere. Both datasets capture the upward propagation of ultra-long QSWs from autumn into winter, highlighting their role in polar vortex displacement and potential changes in the transport of ozone and water vapor.



Zonal mean heat flux [v T*] derived from the QSW components for January in the JAWARA reanalysis (2005-2024; left panel) and UA-ICON free run (10 years; right panel). Black solid lines at 50-60-70 deg N denote the BSR.*

7. Additional use of resources

7.1. University Teaching

In the summer semester of 2026, I taught Dynamics of the Atmosphere within the MSc Physics track Ocean, Atmosphere, and Space at the University of Rostock. As part of this module, I

delivered a weekly seminar on high-performance computing (HPC), comprising nine lectures and practical sessions covering: (1) motivation for HPC, (2) remote computing, (3) Linux fundamentals, (4) the miniWeather code, (5) mapping code to hardware, (6) distributed-memory parallelism, (7) data movement, (8) shared-memory parallelism, and (9) performance analysis.

All students were granted access to DKRZ project 1233, allowing them to gain hands-on experience running and parallelizing code on HPC systems and conducting strong- and weak-scaling experiments. For many students, this was their first experience working in a Linux environment. The practical sessions were very well received, and the students showed considerable enthusiasm for learning about DKRZ's computing infrastructure and the architecture and operation of the Levante supercomputer.

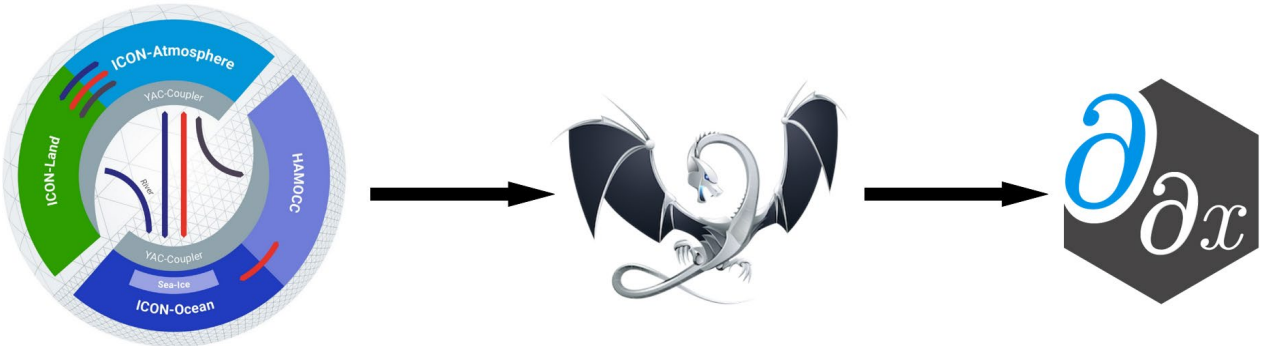
7.2. Public outreach

Like DKRZ, IAP has an Omniglobe for visualizing atmospheric and geophysical processes. Computational resources from this project were used to generate visualizations for public outreach events. These demonstrations consistently attract considerable interest, providing an accessible and engaging way to communicate atmospheric science and the role of numerical modelling to a broad audience.

7.3. Exploring automatic differentiation

We have been investigating the application of automatic differentiation (AD) to ICON and submitted a proposal to Schmidt Sciences. This work was recently presented at the EuroAD workshop in Cambridge. Differentiable programming is attracting growing interest in weather and climate modelling, offering gradient-based approaches to model calibration, optimization, and sensitivity analysis. However, applying AD to large Fortran codebases remains challenging. Traditional AD tools generally rely on source-to-source transformation and the generation of derivative code, often requiring additional tooling and integration into existing build systems. Enzyme offers an alternative by performing AD at the LLVM intermediate representation (IR) level, enabling differentiation to be integrated directly into the compiler workflow with fewer modifications to the original source code.

ICON-XPP is a state-of-the-art Earth system model. Extending it with UA-ICON introduces additional physical processes and constraints associated with the upper atmosphere, whose response to climate forcing can differ substantially from that of the lower atmosphere. We aim to use Enzyme-based AD to quantify parameter sensitivities and enable efficient, systematic calibration of the coupled model. This work would establish a foundation for improving physical parameterizations and, ultimately, for developing differentiable hybrid machine-learning–physics models and enabling online optimization.



Enzyme operates on the LLVM intermediate representation generated from ICON's Fortran code, providing forward- and reverse-mode derivatives without requiring separately maintained tangent-linear or adjoint source code. We initially target self-contained physics parameterizations and scalar tuning parameters, allowing us to quantify local parameter sensitivities before extending toward larger coupled model components.