Usage Report of DKRZ Resources

Project: bb1152 ClimXtreme (subproject bm1159)
Project title: ClimXtreme: Climate Change and Extremes (ClimXtreme)
Project leader: Petra Friederichs, F. Kaspar, J Pinto, U. Ulbrich
Project Funding: BMBF
Reporting period: 11/2023 – 04/2024

Resource bb152	Granted	Utilization	Remaining
Levante CPU nodes (Node hours)	23280	7179	16101
Levante GPU nodes (Node hours)	10000	2500	7500
Levante Storage (TiB)	184	140	44
Archive project (TiB)	52	733	-681
Archive long term (TiB)	2	27	-25
Resource bm1159	Created	a particulation of	- · ·
Resource bilitiss	Granted	Utilization	Remaining
Levante CPU nodes (Node hours)	5170	2116	Remaining 3054
			0
Levante CPU nodes (Node hours)	5170	2116	3054
Levante CPU nodes (Node hours) Levante GPU nodes (Node hours)	5170 10000	2116 2633	3054 7367

Table 1: Used resources at DKRZ (by end of April 2024) in project bb1152 (and subproject bm1159).

During the reporting period from October 2023 to April 2024, work on the ClimXtreme sub-projects was staggered. Some projects officially started in summer 2023, others in winter 2023. Recruitment procedures are still ongoing for some, which leads to varying progress of the work in the sub-projects and the resources used. As a result, not all computing capacities in the bb1152 project were utilized, as not all planned work was started, but due to the major reductions in the last allocation request, the loss of resources was small. However, when all subprojects are starting in the following month the computing time is still needed, and therefore allocated again by some submodules.

In the sub-project bm1159, the use of the joint evaluation system XCES [1] was taken up as planned and increased compared to the first phase, which was primarily visible through more users and diverse evaluations. In particular, the KickOff project in December and the joint work evaluating the flood event in December '23 to January '24 in Germany increased the use of XCES in the project and thus also the use of computing time and storage in bm1159.

In recent months, climate simulations from the former Miklip project [2] have also been archived and are currently being integrated by colleagues at the DKRZ. This is currently leading to an overuse of archive resources, which has already been discussed with the responsible colleagues at the DKRZ.

Scientific activities conducted during the report time

1. Module A – A1 SEVERE

Subproject: A1: Scale Dependent Process Representation and Sensitivity Analysis for Most Extreme Events Subproject leader: Hendrik Feldmann and Joaquim G. Pinto, Institute of Meteorology and Climate Research (IMK-TRO), Karlsruhe Institute for Technology (KIT)

1.1 Usage report November 2023 – April 2024

During the period convection permitting simulations with grid spacing of ~3km were performed with ERA5 forcing to analyze the representation of sub-daily extreme precipitation events detected in observations. A publication regarding the detection efficiency of extreme events from coarse GCM simulations is in preparation. This detection method will be used to identify events with return periods beyond 100-years and perform a regional downscaling (Figure 1).

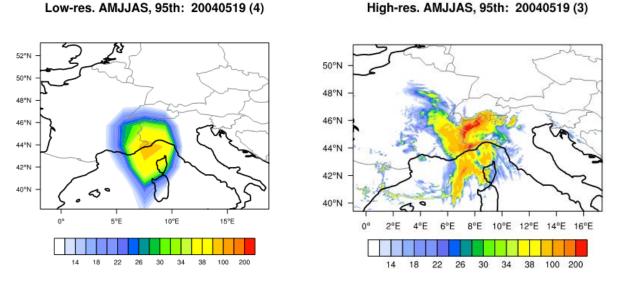


Figure 1: Representation of an extreme precipitation event in MPI-ESM-LR with a grid spacing of ~200 km and downscaled with COSMO-CLM with 3 km grid spacing.

2. Module A – A3 ArcClimEx & A9 ECCES

Subproject:	A3: Linkage between Arctic Climate Change and Weather and Climate Extremes over
	Central Europe
	A9: Climate Change Impacts on Storm Surges in the North Sea
Subproject leader:	A3: Dörthe Handorf (Alfred Wegener Institut), Uwe Ulbrich, Henning W. Rust (FUB)
	A9: Moritz Mathis, Thomas Pohlmann, Bernhard Maver (Uni Hamburg)

2.1 Usage report November 2023 – April 2024

Both projects were part of the first phase of ClimXtreme, which ended in Summer 2023. For finishing phd theses and scientific papers the data and conducted work needed to be available and some computing time was needed for data processing.

3. Module A – A5 DynProHeat (Phase 1) + DesAttHeat (Phase2)

A5: The role of multi-scale dynamical processes in shaping recent and future extreme hea		
waves over Germany		
Andreas Fink ¹ , Joaquim G. Pinto ¹ , Frauke Feser ²		
1) Institute of Meteorology and Climate Research (IMK-TRO), Karlsruhe Institute for		
Technology (KIT), Karlsruhe 2) Institute of Coastal Systems Helmholtz-Zentrum Hereon,		
Geestacht		

3.1 Usage report November 2023 – April 2024

During the reporting period, the focus was on investigating the connection between Central European heatwaves and large-scale disturbances of the climatological, zonal base flow. Earlier results indicate that, in addition to the classic atmospheric blocking by an omega high, the so-called subtropical ridges could play a greater role in the future climate. In order to investigate this question in more detail, the detection algorithm of Sousa et al. (2021) was applied to projections of the CMIP6 MPI-ESM Grand Ensemble (MPI GE; Olonscheck et al., 2023) and the SMHI-LENS (Wyser et al., 2021). The large number of simulated years is suitable for obtaining sufficiently robust statistics even for very extreme heatwaves. It can be seen that both in today's model climate and in projections for a significantly warmer climate (SSP585), heatwaves have the highest intensities when they occur in connection with subtropical ridges (Figure 2a,b). In addition, both models simulate an increased frequency of this type of atmospheric blocking for a future climate under SSP585 (Figure 2c,d).

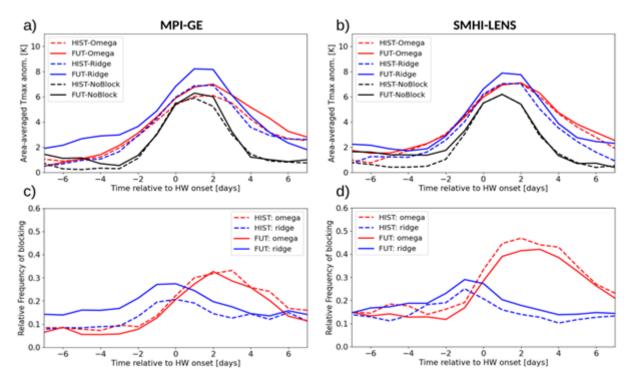


Figure 2: a,b: Intensity of simulated heat waves over Central Europe as a function of atmospheric blocking (red: omega high, blue: subtropical ridge, black: no pronounced blocking) for present-day (dashed line) and future climate under SSP585 scenario (solid line) for MPI-GE (a) and SMHI-LENS (b). c,d: Average proportion of grid points over central Europe with detected omega high or subtropical ridge for the 10% most intense simulated heatwaves for present-day and future climate under SSP585 scenario.

4. Module A – A6 CyclEx

Subproject:

A6: Intensity and structural changes of extreme mid-latitude cyclones change in a warming climate

Subproject leader:

Joaquim G. Pinto¹, Julian Quinting¹, Aiko Voigt² 1) Institute of Meteorology and Climate Research (IMK-TRO), Karlsruhe Institute for Technology (KIT), Karlsruhe 2) Department of Meteorology and Geophysics, University of Vienna, Vienna, Austria

4.1 Usage report November 2023 – April 2024

Dr. Ting-Chen Chen has left the project end of 2023. Svenja Christ started as a PhD student in the project mid-February. Therefore, there have been some delays in the progress. A paper (Chen et al., 2023) on the results of the project has been submitted in the report period.

5. Module B – B1.3 PATTETA

Subproject: B1.3: Process-based attribution of extreme temperatures to anthropogenic drivers Subproject leader: Sebastian Sippel¹, Mareike Kretschmer^{1,2}, Johannes Quaas¹, 1) Leipzig University, Institute for Meteorology, 2) University of Reading, Department of Meteorology

5.1 Usage report November 2023 – April 2024

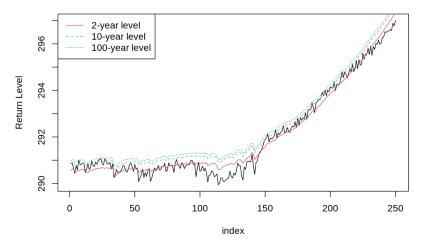
The core objective is to deepen our understanding of future weather extremes, particularly focusing on the climatic drivers behind heat wave changes in Central Europe, including greenhouse gases, aerosols, and atmospheric circulation. Structured into three work packages (WPs), PATTETA aims to:

Assess the impact of greenhouse gases and aerosols on historical to present heat waves (WP1), determine the role of atmospheric circulation in the frequency of extreme heat events and project these findings into future scenarios (WP2), and facilitate the transfer of this knowledge to address practical, application-relevant questions, such as envisioning historical heat waves in future climates (WP3). To achieve these goals, PATTETA utilizes advanced climate modeling techniques, particularly leveraging DAMIP simulations within CMIP6 for WP1 and CESM2 model simulations for WP2 and WP3.

We have started to use resources from early 2024 onwards. Specifically, we prepared and downloaded single forcing large ensemble climate model data for WP1, and we ported and installed the climate model CESM2 on Levante for WP2 and WP3. Because we have mainly focused on model setup and testing, we have not yet used a very large share of our granted resources. However, we are now ready to conduct larger simulations, and hence we anticipate that we will use up our current resources in the next reporting period. We describe the state of the simulations in more detail below:

Download and preparation of single forcing large ensemble data

To analyze the distinct effects of aerosols and greenhouse gases on heat extremes (WP1), we downloaded the large ensemble single forcing model simulations from CESM2 to DKRZ. In single forcing simulations, only one forcing (e.g. anthropogenic aerosols or greenhouse gases) is changed, while all others remain unchanged or all but one are changed (e.g. all but anthropogenic aerosols). We plan to use these simulations to determine the different contributions to global and regional heatwave trends. An initial result is shown in Figure 3.



CESM2 - Ensemble Mean of hottest month over Germany

Figure 3: This figure shows the ensemble mean of all 100 simulations of CESM2-LE over Germany for the period 1850-2100. The return periods are calculated by fitting a Generalized Extreme Value (GEV) distribution with global mean surface temperature as a covariate to the ensemble mean, which is standard in statistical attribution analyses. It appears that the fit underestimates the cooling over Germany in the mid-20th century caused by increased aerosol concentrations over Europe. It also underestimates the strong warming after 2000, which is enhanced by the reduced aerosol concentrations. We plan to quantify these results using large ensemble single forcing simulations (WP1).

Setting up the Community Earth System Model Version 2 (CESM2) on Levante

To use CESM2 for various research questions regarding the attribution of extreme events (WP2 and WP3 in PATTETA), we ported CESM2 to Levante. This was achieved with the help of the DKRZ staff. The CIME environment which is used to set up and perform CESM simulations was configured to run with the compilers which are used on Levante. We carried out some first test simulations. Specifically, we checked the bit-by-bit reproducibility of the model on Levante which is important for our planned experiment design. Besides we did benchmarking tests and tested different options to branch from existing runs with and without perturbations. We also tested how we can branch from simulations that were computed on different computing clusters.

Using CESM2 for circulation nudging experiments

With the aim of using CESM2 for the attribution of extreme events, we started to set up a framework to nudge CESM2 wind fields to ERA5, which has not been done so far. For this purpose, the ERA5 data stored on Levante is transformed to be used as input as nudging files, which requires regridding from pressure to model levels. Initial simulations with forced sea surface temperatures (SST) are set up to test how well the observed surface temperatures and precipitation can be reproduced by nudging to wind fields. Different nudging schemes (nudging frequency, nudging strength and the vertical profile for nudging) are investigated in how well they reproduce observations or create nudging artifacts. An SST input for the simulations at pre-industrial conditions is produced by spatiotemporal detrending of SST observations to be used for the counterfactual simulations. The counterfactual simulations are performed to test whether the circulation patterns observed under climate change produce stable results.

Computing a small CESM2 ensemble for boosting experiments

Besides the above mentioned tests and nudging experiments, we started simulating an ensemble of current climate simulations and pre-industrial control simulations that are required for an in-depth attribution of extreme weather events in current and a counterfactual pre-industrial climate.

6. Module B – B2.4 XPreCCC

Subproject:B2.4: Characterizing EXtreme Precipitation Events under Climate Change ConditionsSubproject leader:Edmund Meredith, Henning Rust and Uwe Ulbrich, FU Berlin

6.1 Usage report November 2023 – April 2024

XPreCCC previously performed ensemble pseudo global warming simulations (Meredith et al., 2022) for a period of high convective activity over Germany. These simulations were the basis of Meredith et al., 2023. At the start of the reporting period, the global warming simulations were repeated using a different warming signal, in order to compare the results with those derived from the previous experiment. These simulations involved creating an 18-member ensemble of 14-day simulations at 0.025° resolution with COSMO-CLM over the COSMO-DE domain. The simulations will presently be analysed with tracking algorithms (Meredith et al., 2022) which were previously developed for Meredith et al. (2023).

7. Module C – C1 CARLOFFF

 Subproject:
 C1: Convective Atmospheres: Linking Radar-based Event Descriptors and Losses From Flash Floods

 Subproject leader:
 Gerd Bürger and Maik Heistermann, Uni Potsdam

7.1 Usage report November 2023 – April 2024

CARLOFFF addresses the classification of atmospheric fields of stability indices (CAPE, CP, TCW of ERA5) over Germany with respect to their potential to excite extreme convective rainfall events, as represented by CatRaRE¹. Since 2023/11 we have been working on allocating CMIP6 runs and adjusting ERA5 fields for use with the coarser CMIP6 resolution. This required the calculation of convective environments from upper level temperature, humidity, and pressure fields. Moreover, the classification was refined to cover the North/South (N/S) and East-West (E/W) classes, and first calibration runs of the shallow and deep classificators were performed.

The corresponding validation skill is shown in Figure 4. It shows for the N/W and E/W classifications the multinomial Ranked Probability Skill Score (RPSS) for all shallow and deep models. One sees that the shallow random forest (TREE) model, with an RPSS of around 0.43, still beats all other methods. An exception, perhaps, is the deep method AlexNet for N/S, whose stochastic optimization renders some variants that even surpass TREE, approaching RPSS values of 5.

¹catalogue of heavy precipitation events (Version 2022.01 exceeding DWD warning level 3 for severe weather

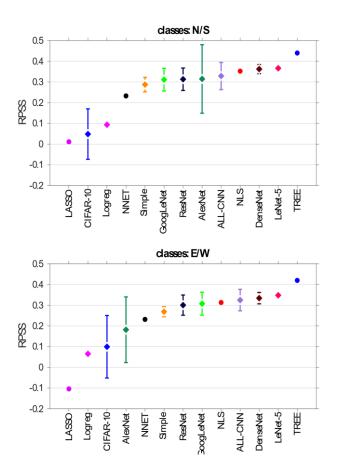


Figure 4: Ranked probability skill score of N/S and E/W classifications of ERA5 with coarser CMIP6 resolution, using extended predictor set.

8. Module D – CoSoDaX

 Subproject:
 bb1159 (D1/D2): Coordination of software and data management for ClimXtreme

 Subproject leader:
 Etor Lucio-Eceiza¹, Deborah Niermann²

 1) Deutsches Klimarechenzentrum Hamburg (DKRZ), 2) Deutscher Wetterdienst Offenbach (DWD)

8.1 Usage report November2023 – April2024

Module D is a supporting module of the ClimXtreme research project and is responsible for the coordination of software and data management (CoSoDaX), especially the development and operation of a central evaluation system for climate extremes (XCES [1]), and the provision and analysis of basic data sets for the evaluation of climate extremes, as well as the support of software developments for the investigation of extreme events and the maintenance of existing software. XCES is based on Freva (Kadow et al., 2020), a scientific software framework for high performance computing, equipped with a standardized model database, a programming interface and a history of evaluations, maintained and updated by the Climate Informatics and Technologies (CLINT [3]) group at DKRZ. One of the primary goals of Module D is to build up a reasonable database for the joint project, accessible through XCES. Based on the data from the former MiKlip project [2], this data collection has been progressively expanded during the first phase of ClimXtreme. In the current phase we focus mainly on the provision of near-realtime data, which results in a constantly growing storage requirement in order to keep the data records up to date. Although the vast majority of the data is linked from the /pool/data, a significant amount of it is hosted under the joint project bm1159 (around 300 TB). An overview of the data types integrated in the system and hosted with resources of bm1159 (joint project of main bb1152) is given in Figure 5. Almost all of the available workspace storage is being used (396 out of 408 TiB or 97% of usage). All data coming from /pool/data (e.g. CMIP6, CORDEX, etc.) are updated (re-crawled) into XCES every week to keep the databrowser as up to date as possible. In addition, special datasets such as HYRAS 1km-de and ERA5 are updated (including standardisation and crawling) every 2 days. These routines are scheduled via scrontab, which uses the project's computing resources, so a significant

amount of computing is devoted to this (about 40%, more than the planned 10%). The standardisation of ERA5 is used by other Freva sister instances (regiklim, gems, freva) and a larger community of users within the DKRZ.

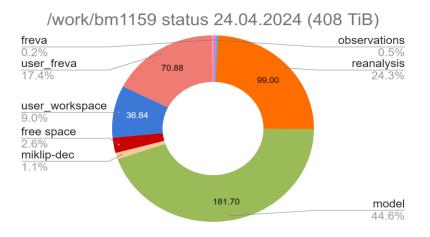


Figure 5: Storage demand (TiB) of different data types under /work/bm1159/XCES/, hosted in the ClimXtreme project bm1159 and percentage of data according to their type.

XCES grants a flexible incorporation of verification routines (plugins). These analysis tools are being developed by Modules A-C with the assistance of Module D, or by Module D itself to fulfill the needs of the project and be used by any member of the Consortium. Within the project 11 plugins have been developed (for an overview see Table 2). Additionally, 12 plugins were inherited from the former MiKlip project or ReglKlim sister project.

The goals of the plugins are very diverse, from the calculation of atmospheric circulation regimes by K-means clustering (e.g. Figure 6 left), to calculation of Intensity-Duration-Frequency curves at certain stations (e.g. Figure 6 right).

plugin	topic	project
CLIMPACT_SCI	calculation of ET-SCI climate extreme indices	C1
COOC	Co-occurrence of extreme events	C1
getCDCstation	ingestion of station observations from DWD CDC	D1
IDF	Intensity Duration Frequency curves	B2.5
PCA*	Principal Component Analysis based on XEOFS library	B3.7
PLL	Optimization of Pairwise Log-Likelihood function	B3.1
PSI	calculation of the Precipitation Severity Index	A1
REALISTIC	reanalysis / observation data comparison	D1
Regimes	Identification of circulation patterns	A3
TPDM	Tail Pairwise Dependence Matrix	B3.1
trendtest*	linear trends applying the T-test for significance	B3.7

Table 2: Overview of plugins developed during ClimXtreme (recent additions with *) project and a short description of their functionality.

These plugins are hosted and run through XCES and are available to the entire ClimXtreme community. During the period 2023.11-2024.04, more than 4,600 plugin calls have been made, so the amount of storage allocated to outputs has grown steadily. XCES users currently use close to 110 TiB between plugin outputs, data indexed back to XCES, and their own workspace. Both plugins developed within and databases accessible through XCES have been used for several event studies and publications within the project.

The total CPU usage between data (around 40%) and plugin runs (around 60% between actual usage and plugin bugfix and development) adds to close to 2,300 node hours, that is, more than 44% of the granted resources for the complete 2024 period (133% of the granted resources for Q1 so far). These utilized resources correspond to the expected use of the XCES after the kickoff of the project last December and the associated increased cooperation and evaluations that have begun.

An adjacent line of research of CLINT is focused on the application of AI/ML methods (Kadow et al., 2020) to tackle a variety of climate science related topics, with a direct usability through XCES (i.e., data and plugins) in mind. The research group has been further developing these methodologies under HLRE 4's GPU cores. Examples of recent lines of research are the following: infilling of observations for data assimilation for the improvement of numerical climate prediction systems in relation to extremes; prediction of extremes in temperature measurements and digital twins; and the creation of a classifier tool for climate model seasonal predictions of extremes (the later has also extensively used decadal prediction plugins developed within MiKlip that were re-adapted during the last period of Phase1, and that will be needed in the upcoming Coming Decade Freva sister project). More than 27% of GPU resources have been used so far, a little below the allocated ones for Q1.

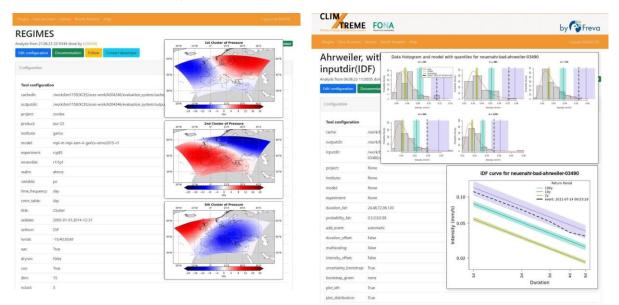


Figure 6: (left) 1,2 and 5th cluster modes for a selected region, time period and gridded sea level pressure dataset via REGIMES plugin, developed at XCES by Module A3. (right) Evaluation of Intensity-Duration-Frequency curves at Neuenahr Bad Ahrweiler site showing its more extreme historical event at 2021.07. Via IDF plugin, developed at XCES by Module B2.5.

9. Project related publications

- Becker, F. N., Fink, A. H., Bissolli, P., & Pinto, J. G. (2022): Towards a more comprehensive assessment of the intensity of historical European Heat Waves 1979-2019, Atmospheric Science Letters, 23(11), e1120.
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- Chen, T.-C., C. Braun, A. Voigt, and J. G. Pinto (2023), Changes of intense extratropical cyclone deepening mechanisms in a warmer climate in idealized simulations, Submitted to Journal of Climate, Under review.
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- Franco-Díaz, A. Feldmann, H., Suarez-Gutierrez, L. Müller, W., Pinto, J.G., 2023: Extreme precipitation events in the MPI-ESM Grand Ensemble. (In preparation)
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