FINAL REPORT for a Simulation Project on the Supercomputer JUROPA/JURECA

Period: Nov 2015 – Oct 2016

PROJECT TITLE: WASCAL – Regional climate simulations for West Africa

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1 Final report for project WASCAL

In our application for computational resources on JURECA for the period 11/2015 to 10/2016, we proposed two separate tasks for computation on JURECA. Firstly, we proposed to finalise the long-running high-resolution regional climate simulation experiment with WRF on JURECA, for which approximately 850 000 core-hours were required. The progress and current status of this task is summarised in Sect. 1.1. Secondly, we presented a novel atmospheric model, the Model for Prediction Across Scales Atmospheric core (MPAS-A), which is based on an irregular, variable-resolution mesh, and proposed to conduct a seasonal forecasting and climate research experiment using this model. For this experiment, we applied for 3 185 000 core-hours.

In total, we were granted 1 350 000 core-hours for this period, which means that not all of our planned work could be accounted for. The feedback of the reviewers on our proposal for computing time stated clearly the importance to finalise the high-resolution regional climate simulations with WRF. Hence, we concentrated our efforts on this task first, leaving about 500 000 core-hours for the MPAS-A experiment. These resources were insufficient to conduct the proposed experiments with MPAS-A on JURECA only. Since the inter-comparability of the results is crucial and the usage of different HPC systems in general leads to different results for identical model runs, we concluded to not perform the suggested MPAS-A work on JURECA and use parts of the remaining resources for development work, in particular on the parallel performance, of the MPAS-A core (Sect. 1.2).

1.1 High-resolution regional climate simulations

The regional climate modelling experiment in WASCAL is a continuous project over several years. As described in the applications 2013, 2014 and 2015, this project focusses on the long-term high-resolution regional climate simulations for West Africa. The overarching goal of this part of WASCAL is to produce simulations of unprecedented resolution and accuracy for a large fraction of the 21st century and an area covering the whole of West Africa. It therefore exceeds and complements recent studies and large-scale projects such as CORDEX. The past has shown that in order to address the uncertainties in regional climate projections, caused by the diverging climate change signals in the driving global model data and the different regional models, an ensemble approach is best suited.

Our ensemble consists of a combination of three global circulation models (GCMs) with three regional climate models (RCMs) for the green house gas scenarios rcp4.5. The choice of rcp4.5 only was made because of limited computational resources and is based on the fact that (a) the differences between rcp4.5 and rcp8.5 become apparent only after 2040, and (b) that the rcp4.5 scenario – to current knowledge, in particular after the COP21 agreement was made in Paris in December 2015 – is the most realistic scenario. The selected GCMs, on the other hand, cover the extremes in temperature and precipitation of the GCM ensemble used in CORDEX and span a larger range of conditions until about 2060 than the two scenarios. Further, control runs using re-analysis data are included for model verification and bias correction. At the end of this project, we will therefore be able to provide an ensemble of 3×3 regional climate projections at high temporal (3-hourly data) and spatial (12 km) resolution over the whole of West Africa. Table 1 summarises the different driving GCMs and RCMs used for the WASCAL ensemble experiment.

As described in the previous applications for computing resources, the model experiments are split across several HPC facilities in Germany due to the high demand of computational resources. Likewise, accompanying studies on the evaluation and optimisation of the regional models employed here and on fully coupled atmospheric-

Table 1: Re-analyses and global circulation models (earth system models) used as forcing data for the long-term regional climate simulations, and regional climate models used to conduct the ensemble experiment. The characteristics of each forcing model for Africa are taken from [10].

GCM/ESM	**Characteristics for West Africa**	**Reference**
ERA-Interim	re-analysis data, “perfect atmosphere”	Dee et al.(2011) [3]
MPI-ESM MR	temp and precip close to multi-model mean	Stevens et al.(2013) [13]
HadGEM2-ES	warmer and drier than multi-model mean	Collins et al. (2011) [2]
GFDL-ESM2M	colder and wetter than multi-model mean	Dunne et al. (2012) [5]
RCM	**Model configuration for West Africa**	**Reference**
WRFV3.5.1	Klein et al. (2015) [9]	Skamarock et al. (2008) [12]
CCLM 4.18	Panitz et al. (2014) [11]	Baldauf et al. (2011) [1]
RegCM4	Sylla et al. (2011) [14]	Giorgi et al. (2012) [7]

hydrological models (e. g., WRF-Hydro) are conducted elsewhere. It is important to note, however, that these results and our preparatory work on ideal model configurations for the different RCMs have found their way back to the model developers and to the scientific community, through publications and conference presentations (see also Sect. 2). Table 2 summarises the status of the ensemble simulation experiment before the running application period (Oct. 2015) and now (Aug. 2016), which highlights the progress that has been made with WRF on JURECA and with CCLM on the Steinbruch Center for Computing (SCC) ForHLR1 supercomputer.

The JURECA HPC and its successor JUROPA were used exclusively for the long-term regional climate simulations with WRF. To ensure consistency between the model results on JUROPA and JURECA, we repeated a 10-year simulation experiment, previously conducted on JUROPA, on JURECA. The differences in the results were similar or smaller than those between JUROPA and DKRZ Blizzard. Since the experiments conducted on JURECA were using a different forcing model (HadGEM2-ES) than those on JUROPA (GFDL-ESM2M and MPI-ESM MR) and Blizzard (ERA-Interim), we decided to accept these small differences.

As the WRF simulations are finished, we currently do not plan to conduct further runs on JURECA in the coming application period. The CCLM experiments will be continued on ForHLR1 for the sake of the above-mentioned consistency. While the WRF and CCLM experiments were/are conducted by researchers at KIT/IMK-IFU, the RegCM experiments are in the hands of the WASCAL Competence Center in Ouagadougou, Burkina Faso. They were planned to be run on the German Climate

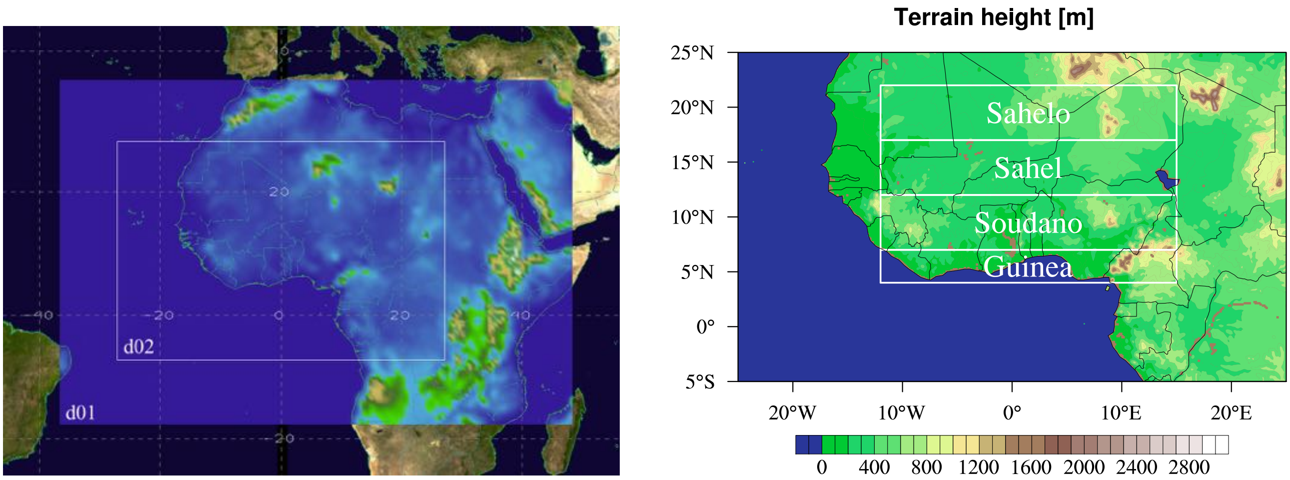

Figure 1: (left) Domain setup for WRF, d02 at $12\,\mathrm{km}$ resolution with $496 \times 331 \times 40$ grid points nested in nested in d01 at $60\,\mathrm{km}$ resolution with $156 \times 107 \times 40$ grid points; (right) model topography of the analysis area and definition of distinct agro-climatical zones used for the analysis.

Computing Center (DKRZ) Mistral supercomputer, but have not yet been initiated. With the installation of its own HPC system in 2016, the Competence Center will most likely decide to conduct these simulations directly on their own system.

An in-depth analysis of the WRF model results with particular focus on the West African Summer Monsoon and its dynamics and precipitation characteristics is ongoing and we expect to submit one or two comprehensive articles within the next 6–9 months. An analysis of the CCLM control runs is already under review [4]. As shown in last year's report, our preliminary results suggested that the higher resolution used in our simulations and the optimised model setup for the region lead to improvements compared to existing data sets from, for example, the CORDEX project [6]. In particular, we found improvements for the modelled annual cycle of precipitation and for the timing of the onset and cessation of the rainy season.

In this report, we focus entirely on the now completed set of WRF simulations to illustrate the differences between the different forcing data sets and their respective projections of future climatological conditions. As a reminder, Fig. 1 displays the model topography of the inner 12 km WRF domain and selected agro-climatical zones following a South-North gradient in precipitation used for the analysis.

Figures 2–5 in Sect. 4 display the current results of our low-resolution (60 km) and high-resolution (12 km) WRF simulations and from UDEL observations [15] for the historical period 1980–2010 and for the projections 2020–2050 and 2070–2100 for

Table 2: Design and progress of the WASCAL high-resolution regional climate ensemble.

GCM/ESM	RCM	Experiment	HPC	Oct. 2015	Aug. 2016
ERA-Interim	WRFV3.5.1	control	DKRZ Blizzard	completed	completed
	CCLM 4.18	control	DKRZ Blizzard	completed	completed
	RegCM4	control	DKRZ Mistral	not yet started	not yet started
MPI-ESM MR	WRFV3.5.1	hist.	FZJ Juropa	completed	completed
	CCLM 4.18	hist.	SCC ForHLR1	completed	completed
	RegCM4	hist.	DKRZ Mistral	not yet started	not yet started
	WRFV3.5.1	rcp4.5	FZJ Juropa	completed	completed
	CCLM 4.18	rcp4.5	SCC ForHLR1	in progress	post-processing
	RegCM4	rcp4.5	DKRZ Mistral	not yet started	not yet started
GFDL-ESM2M	WRFV3.5.1	hist.	FZJ Juropa	completed	completed
	CCLM 4.18	hist.	SCC ForHLR1	not yet started	not yet started
	RegCM4	hist.	DKRZ Mistral	not yet started	not yet started
	WRFV3.5.1	rcp4.5	FZJ Juropa	completed	completed
	CCLM 4.18	rcp4.5	SCC ForHLR1	not yet started	not yet started
	RegCM4	rcp4.5	DKRZ Mistral	not yet started	not yet started
HadGEM2-ES	WRFV3.5.1	hist.	FZJ Jureca	pre-processing	completed
	CCLM 4.18	hist.	SCC ForHLR1	not yet started	not yet started
	RegCM4	hist.	DKRZ Mistral	not yet started	not yet started
	WRFV3.5.1	rcp4.5	FZJ Jureca	pre-processing	completed
	CCLM 4.18	rcp4.5	SCC ForHLR1	not yet started	not yet started
	RegCM4	rcp4.5	DKRZ Mistral	not yet started	not yet started

Notes. The control runs are conducted for the period 1979-2014. The historical runs are generated for the period 1979-2005 and extended by the rcp4.5 runs until 2010. This approach allows us to derive statistics for the climatological reference period 1980–2010, as redefined by the WMO in 2015. Future projections are calculated at least for the periods 2019–2050 and 2069–2100 to provide similar 30-year windows for mid and end of the 21st century.

rcp4.5. Starting with historical surface temperature, we find that the re-analysis runs WRF-R underestimate observed temperatures northwards of 15°N, and overestimate them between 10°N and 15°N. Closer to the Coast of Guinea, the agreement between UDEL and WRF-R is improved. A similar behaviour, with overall lower temperatures and a better match of the observations, can be found for the historical runs using MPI-ESM MR forcing data (WRF-M). The mean annual temperature as well as the annual cycle of the remaining WRF-G and WRF-H runs are substantially cooler by up to 2°C for WRF-H and 3°C for WRF-G. The difference between the low- and high-resolution runs is smaller than between the different forcing data sets.

With respect to precipitation, we observe a different behaviour: With the exception of the northern Sahel and Sahelo area, the WRF-G run reproduces the observed precipitation amount and pattern best, followed by WRF-H. The latter is showing highest accuracy among all runs in the northern areas. The re-analysis runs are showing good agreement in the northernmost areas, too, but overestimate precipitation towards the south-east of the domain (i. e. in the Niger Delta). The WRF-M run, best among all models in terms of temperature, overestimates precipitation most. In general, the low-resolution runs tend to produce less precipitation than the high-resolution runs, which improves the model performance for WRF-M and in parts for WRF-R, and deteriorates it for WRF-H and WRF-G. As suggested by Fig. 3, we suspect that on smaller spatial scales, and in particular in complex terrain such as the coast line, the added value of the high-resolution runs becomes more apparent.

Our findings briefly summarised here stand in contrast to the conclusions drawn in [10], which classify HadGEM2-ES as warmer and drier, GFDL-ESM2M as colder and wetter, and MPI-ESM MR as close to the multi-model mean. We attribute this to the fact that in [10], the raw GCM model output was analysed, while we are facing the output of WRF that uses the respective model as forcing data. The somewhat opposing characteristics, in particular far away from the domain boundaries, might be due to the necessarily different pre-processing steps taken for each of the GCMs, the differences in their grid size and design as well as in their prescribed properties such as land-use classification, albedo, etc.

Lastly, we take a quick look on the projected changes in temperature and precipitation. For the sake of visibility, only the high-resolution runs are displayed. All models predict an increase in surface temperatures by up to 2°C (WRF-M, WRF-G) or up to even 3°C (WRF-H), with the strongest increase in the Sahel and Sahelo areas and further north. Nearly no changes can be seen in the seasonal cycle of surface temperatures, i.e. the entire cycle is shifted to higher temperatures. Similarly, all models predict increasing annual rainfall on average with different spatial signals: While WRF-M predicts the smallest increase in rainfall, mainly in the Soudano area, and a slight decline further north-east, WRF-G exhibits an increase in precipitation mostly in the Guinea and the Soudano areas. WRF-H shows a similar spatial distribution as WRF-G, but with an overall larger amplitude of up to 200 mm/a by the end of the 21st century.

1.2 MPAS-A performance improvements

As discussed before, we focused on the improvement of the numerical, parallel performance of MPAS-A based on the results of our extreme scaling experiment conducted in 2015 on JUQUEEN and summarised in a recent publication [8]. These tests at extreme scale, employing between 4 and 24 racks on JUQUEEN (i. e. up to 458 752 cores) for a global, regular 3km mesh with more than 65 Mio. grid cells, revealed in particular two bottlenecks that need to be addressed in order to perform large-scale runs efficiently on current and next-generation supercomputing facilities: parallel I/O and model initialisation. While the details are beyond scope of the current report, we briefly discuss these two aspects and steps taken to address them.

To improve the I/O performance in massively parallel applications, an alternative I/O layer was implemented in the MPAS framework. This I/O layer employs the SIONlib library developed at FZJ to read and write internal data (initial conditions, restart files), but also to write model output files. To convert these into a common format (pnetCDF, netCDF4), a post-processor core for MPAS was developed alongside, which can run on a smaller number of nodes and allows the atmospheric model to perform the dynamical integration at maximum performance.

The bottleneck in the model initialisation lies in an initial bootstrapping process, during which every MPI task identifies which cells to exchange with which neighbours. This step scales approximately quadratically with the number of MPI tasks and took more than 20 minutes to complete on 24 racks of JUQUEEN. A promising approach therefore is to implement a hybrid MPI+OpenMP parallelisation in MPAS-A, which reduces model initialisation times and communication patterns and, ideally, leads to a similar speedup of the dynamical solver (time integration) than if we were using a larger number of MPI tasks.

We have started to address both aspects in project funded by the "Kompetenznetzwerk für wissenschaftliches Höchstleistungsrechnen in Bayern (KONWIHR)" of the Bavarian Academy of Science. In this development phase, JURECA was used for medium-size scaling experiments alongside with LRZ's SuperMUC. Until now, we could speedup the write performance using SIONlib by a factor of 10 relative to pnetCDF (60 relative to netCDF4). Our hybrid parallelisation led to similar performances of the dynamical solver for 16×1, 8×2 and 4×4 (MPI×OpenMP) tasks on a 16-core machine, while significantly reducing the model initialisation time.

2 Publications from project WASCAL

The following list summarises publications that are directly or indirectly related to our project on JUROPA/JURECA through, for example, usage of our data or our model optimisations:

- Arnault, J., Wagner, S., Rummler, T., Fersch, B., Bliefernicht, J., Andresen, S., Kunstmann, H. (2016): Role of Runoff-Infiltration Partitioning and Resolved Overland Flow on Land-Atmosphere Feedbacks: A Case Study with the WRF-Hydro Coupled Modeling System for West Africa. J. Hydrometeor., 17, 1489–1516, 10.1175/JHM-D-15-0089.1
- Arnault, J., Knoche, R., Wei, J., Kunstmann, H. (2016): Evaporation tagging and atmospheric water budget analysis with WRF: A regional precipitation recycling study for West Africa, Water Resour. Res., 52, 1544–1567, 10.1002/2015WR017704
- Heinzeller, D., Duda, M.G., Kunstmann, H. (2016): Towards convection-resolving, global atmospheric simulations with the Model for Prediction Across Scales (MPAS): an extreme scaling experiment. Geoscientific Model Development, 9, 77–110
- Klein, C., Heinzeller, D., Bliefernicht, J., Kunstmann, H. (2015): Variability of West African monsoon patterns generated by a WRF multi-physics ensemble, Climate Dynamics, 10.1007/s00382-015-2505-5
- Klein, C., Bliefernicht, J., Heinzeller, D., Gessner, U., Klein, I., Kunstmann, H. (2016): Feedback of observed interannual vegetation change: a regional climate model analysis for the West African monsoon. Climate Dynamics, 10.1007/s00382-016-3237-x

3 Ph.D. theses completed within project WASCAL

The following theses were completed in 2016 with contributions from our project through, for example, usage of our data or our model optimisations:

- Cornelia Klein, University of Augsburg, Germany: Uncertainties from above and below - regional climate downscaling of the West African monsoon
- Edward Naabil, Federal University of Akure, Nigeria: Moldeing the Climate and Hydrology of the Tono Basin in Ghana, West Africa

4 Graphics suitable for the general public

Figures 2–5 on pages 11–14 display selected results of our ensemble modelling experiment obtained thus far and can be used for presentation to the general public. We can provide the full PDF images and more detailed descriptions if required.

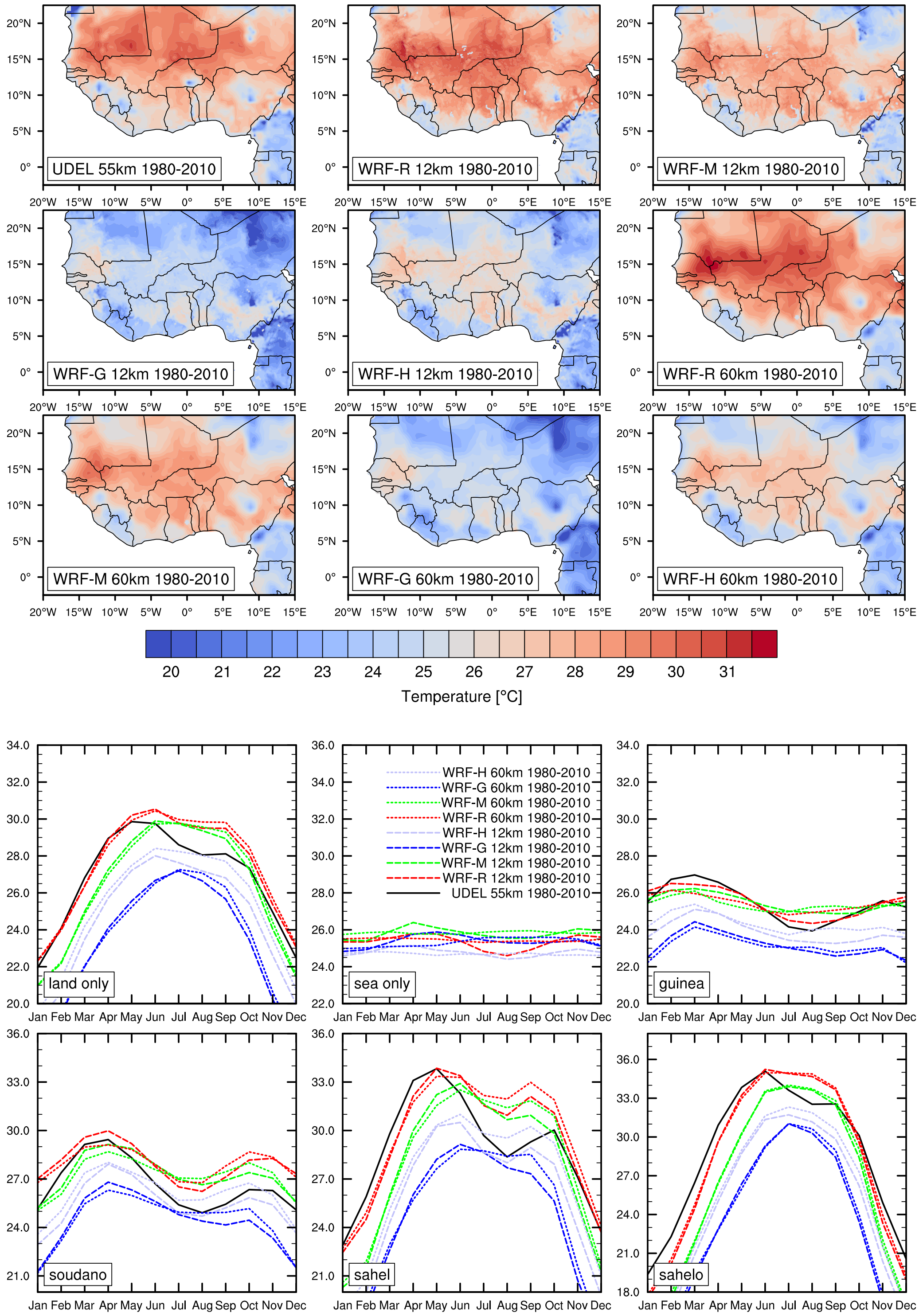

Figure 2: (top) Annual mean surface temperature and (bottom) mean annual cycle of surface temperature 1980–2010 of the WASCAL low-/high-resolution regional climate simulations and UDEL observational data. WRF-R: WRF + ERA-Interim, WRF-M: WRF + MPI-ESM, WRF-G: WRF + GFDL-ESM2M, WRF-H: WRF + HadGEM2-ES, UDEL: University of Delaware.

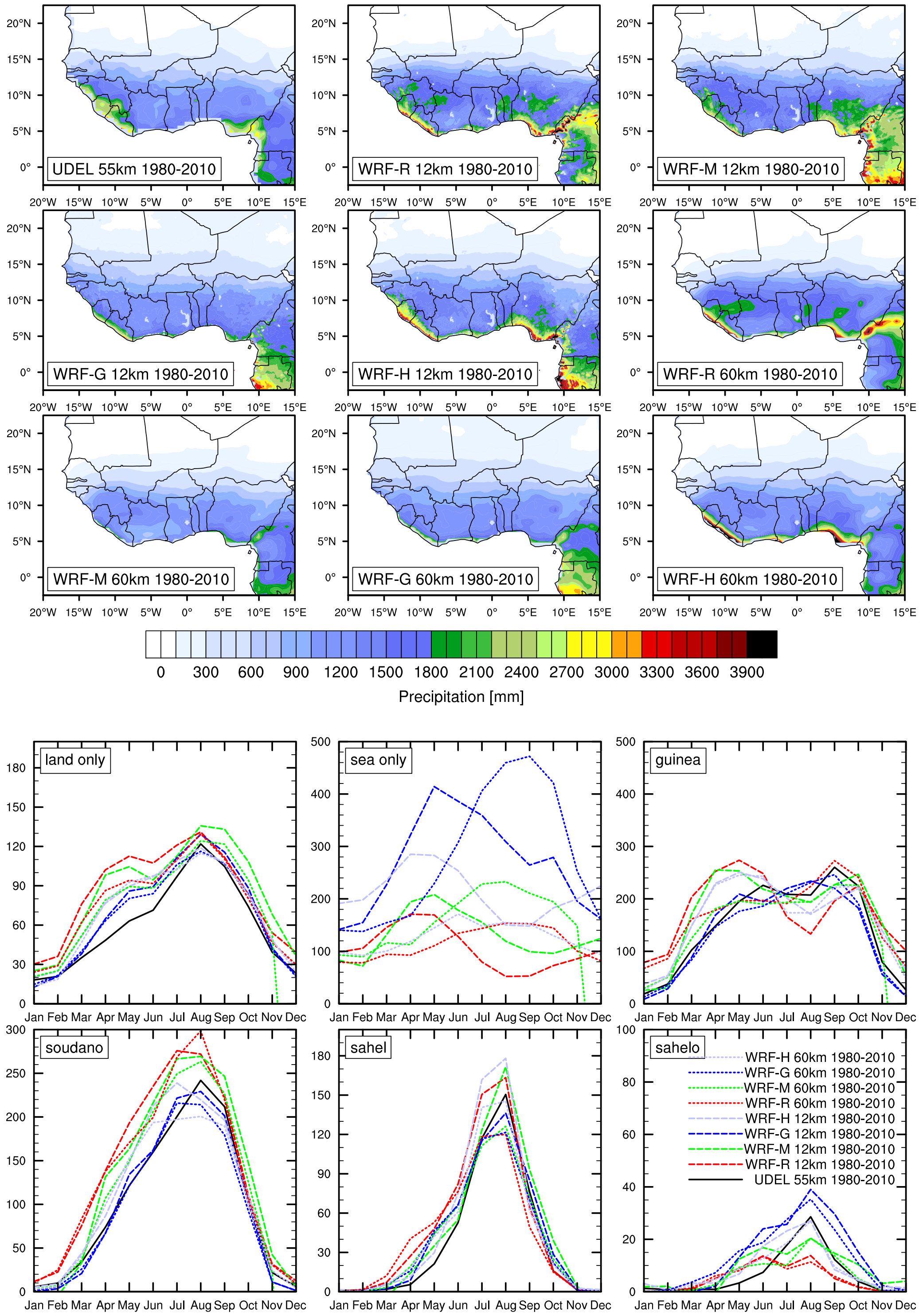

Figure 3: (top) Annual precipitation and (bottom) mean annual cycle of precipitation 1980–2010 of the WASCAL low-/high-resolution regional climate simulations and UDEL observational data. WRF-R: WRF + ERA-Interim, WRF-M: WRF + MPI-ESM, WRF-G: WRF + GFDL-ESM2M, WRF-H: WRF + HadGEM2-ES, UDEL: University of Delaware.

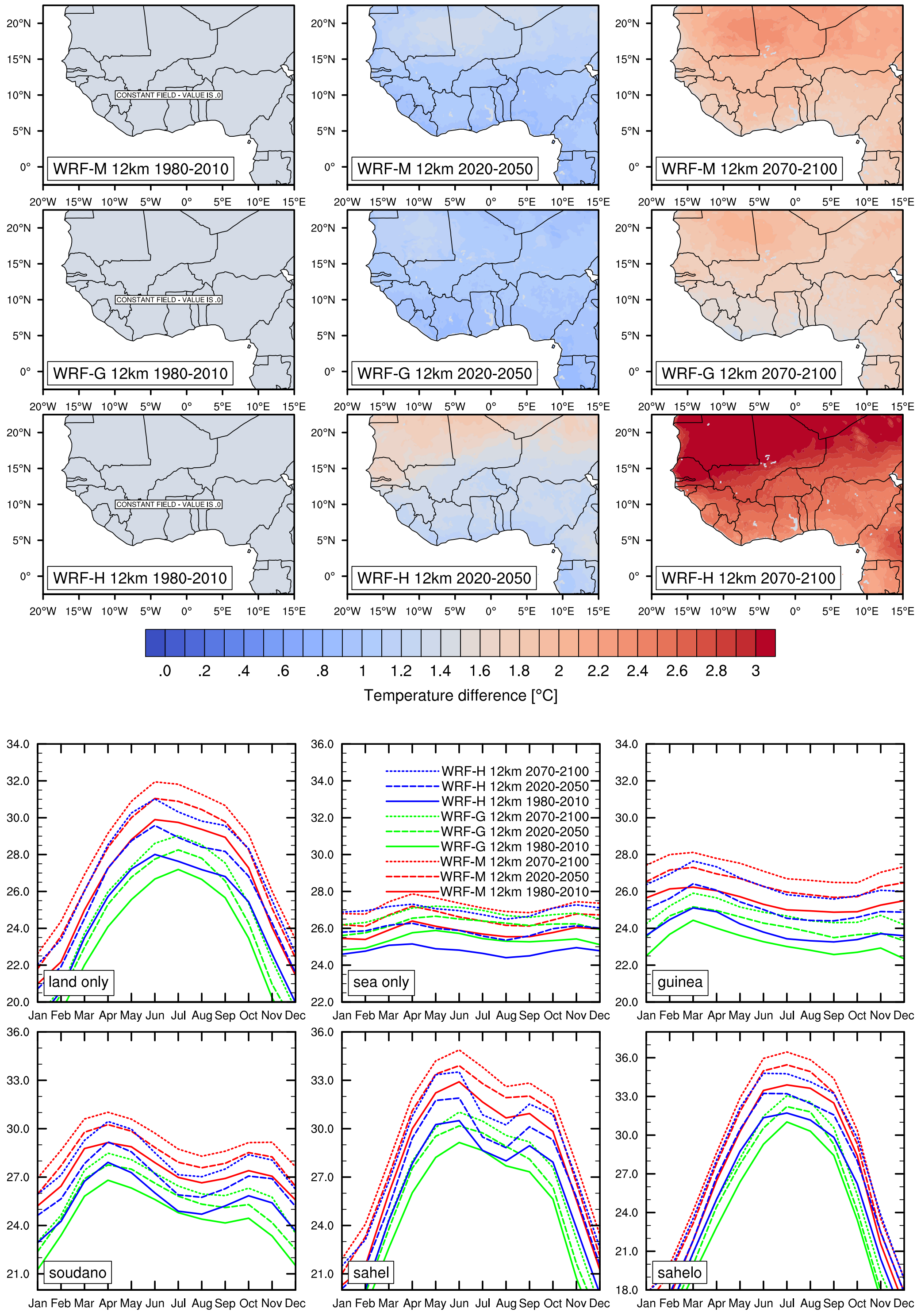

Figure 4: (top) Change in annual mean surface temperature compared to the reference period 1980–2010 and (bottom) mean annual cycle of surface temperature of the WASCAL high-resolution regional climate simulations. WRF-M: WRF + MPI-ESM, WRF-G: WRF + GFDL-ESM2M, WRF-H: WRF + HadGEM2-ES.

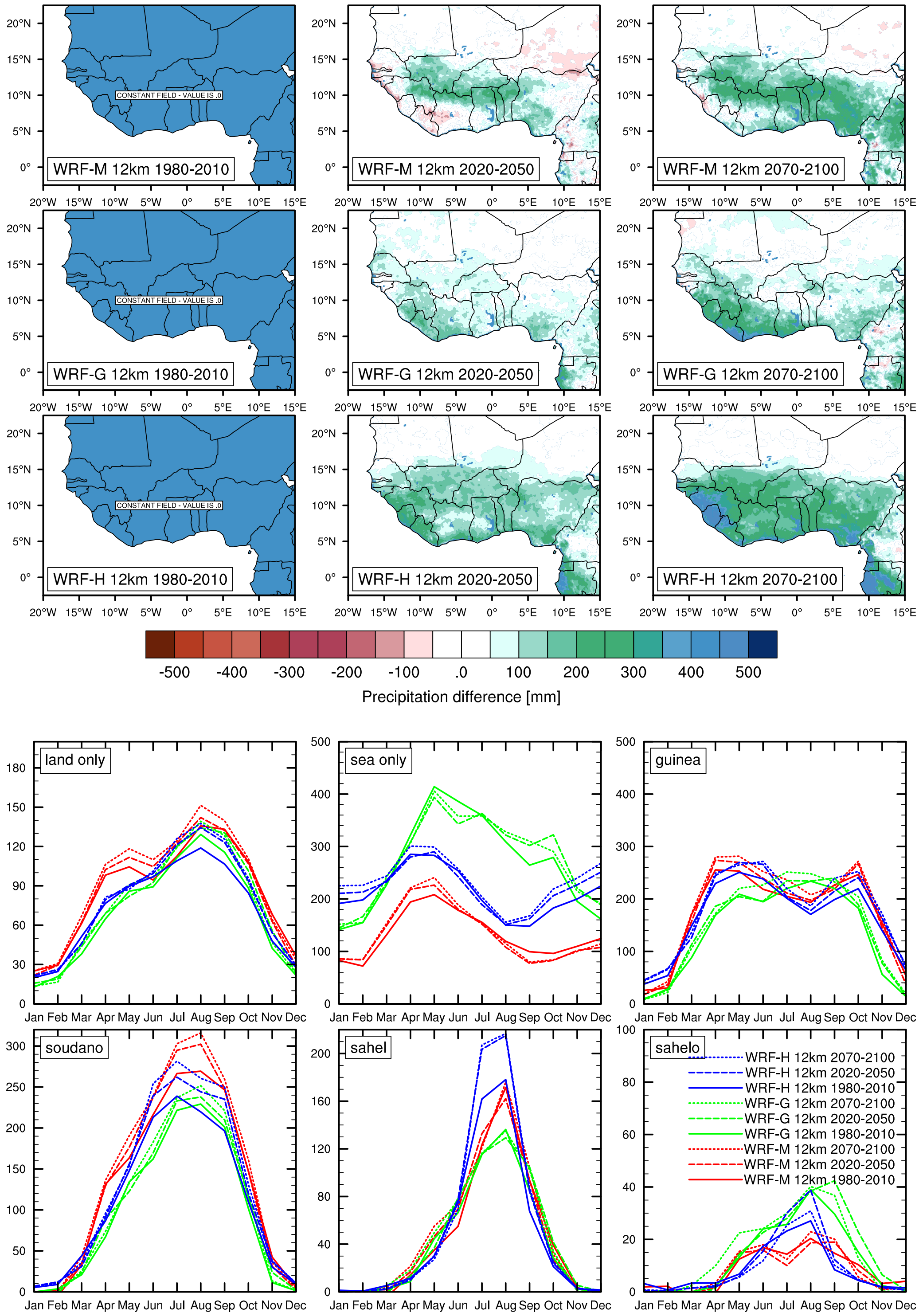

Figure 5: (top) Change in annual precipitation compared to the reference period 1980–2010 and (bottom) mean annual cycle of precipitation of the WASCAL high-resolution regional climate simulations. WRF-M: WRF + MPI-ESM, WRF-G: WRF + GFDL-ESM2M, WRF-H: WRF + HadGEM2-ES.

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