

# PalMod - Paleo Modeling

From the Last Interglacial to the Anthropocene -Modeling a Complete Glacial Cycle

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PalMod is grateful for the computing time granted in 2017. While each PalMod Working Group (WG) submitted a proposal separately, this report summarizes the work of all four work packages within PalMod:

WG1 (project 989)	Physical System
WG2 (project 1030)	Biogeochemistry
WG3 (project 1029)	Synthesis and Analysis of Proxy Data
WG4 (project 993)	Optimization of Quality and Performance

Within 2017 we got 1.3 Mil. node hours granted. By end of October (2 months left) we used app. 83% of the resources. Unfortunately, some resources couldn't be used due to delays in personal support or delays in model development. Please find more details in our reports.

As the first phase of PalMod is devoted to develop earth system models and to identify and investigate feedbacks and processes necessary to successfully simulate the last deglaciation, the number different model versions (32) within PalMod is large. This is due to the fact, that PalMod follows a somehow modular approach with its key advantages to overcome unnecessary dependencies between the different working groups due to ongoing development. So, (i) everybody can start immediately with the tools on hand, (ii) there are only minor dependencies between the working groups, and (iii) the range of investigated models / coupling strategies is much larger, which is a benefit to investigate a larger model-space.

As we are still in a model development-phase we are just on the way that first results are published, but several papers are in submission or in preparation.

Each working group summarizes their scientific progress and their results independently. Please find the 4 reports in the following sections.

#### Project: 989

# Project title: Long transient simulations of the last deglaciation (last 30,000 years) and the development of lithosphere and ice sheet models in the framework of PalMod Working Group 1, Physical System

Project lead: Gerrit Lohmann

Report period: 2017-01-01 to 2017-12-31

We report on our modeling efforts on Mistral during the first 10 months of the allocation period 2017, covering proposed simulations with MPI-ESM, PISM, ISSM, VILMA, CCLM, and AWI-CM. During this time period, the project had 28,029 unused node hours at the end of the third quarter. This was caused by unforeseen long waiting times of the project's simulations on the queue.

At the KIT, the model setup of the regional climate model COSMO-CLM, optimized for simulations of Arctic regions, was driven with ERA-Interim data at 0.7° resolution for the present-day period (1995-2015). The surface mass balance was computed, and has been inferred to be realistic for the Greenland Ice Sheet (GrIS). The optimized model was also driven by a first set of GCM present day climate simulations (MPI-ESM). Due to the low resolution of driving data, a two-step-nesting was needed. Estimated surface mass balance for present day simulations (2000-2004) driven with GCM data shows promising results (Fig. 1). The application for LGM (21ka) data is currently in progress.



# SMB 2000-2004

**Fig. 1:** Surface mass balance based on the optimized 0.22° model driven with MPI-ESM-LR data (2000-2004).

MPI-Met and GFZ Potsdam collaborated to couple the ice sheet model mPISM and the GIA model VILMA bidirectionally. Based on this setup, test simulations were performed for the last deglaciation. Climatic boundary conditions for these simulations were based on 12 steady-state MPI-ESM simulations, processed with the new Energy Balance Model (EBM). After several adjustments and tuning of mPISM as well as the EBM, a reasonable deglaciation of the Northern Hemisphere was obtained. Depression of the bedrock leads to formation of massive lakes at the southern flanks of the retreating ice sheets (Fig. 1).

Massive surges from the ice sheet into these lakes strongly contribute to the deglaciation. Coupling and tuning of the models took longer than previously expected. With adjustments in the mPISM we were able to reduce the computational cost by a factor of 10. First tests of modeling the deglaciation in MPI-ESM with prescribed ice sheets (WG4) are promising. Both the coupling from the climate model to the ice sheets as used in the simulations presented here, as well as the coupling back from ice sheets to the climate model, are ready for the first fully coupled test experiments.



Fig. 2: Ice sheets and bedrock relative sea level changes in a deglacial test experiment. The vertical axis is exaggerated by a factor of 100. Areas below sea level are shown as flooded in dark blue. The colors on the ice show the combined surface and basal mass balance. The isolines mark bedrock / relative sea level changes. Greenish lines mark bedrock depression / relative sea level rise, brown lines mark bedrock uplift / relative sea level fall. White marks ±0m, light color lines ±50m, dark color lines multiples of ±100m. Notice the strong melt on the ice shelves in the periglacial lakes in the isostatically depressed areas south of the big ice sheets.

At the AWI paleoclimate dynamics group, in PalMod-1-3-TP3, the methodology with respect to transient modifications of e.g. orography and freshwater perturbations for the transient simulations has been further improved. Due to technical problems and the pending update of MPI-ESM to the CMIP6-version, the target of running the transient deglacial simulations could not yet be fulfilled, since it is planned to run these simulations with a stationary CMIP6 MPI-ESM code-version. Therefore, the computational resources were utilized for various key sensitivity studies that sample the phase space of MPI-ESM and AWI-CM with respect to the impact of freshwater perturbations and the glacial climate forcing; one example is shown below (Fig. 3). Furthermore, a novel synthesis of critical boundary conditions (ice sheet topography and atmospheric CO2 concentrations) for the stability of the AMOC (Zhang et al. 2017) has been established. This synthesis shows that high continental ice sheets (Zhang et al., 2014) as well as high atmospheric CO2 (Zhang et al., 2017) concentrations lead to a strong monostable AMOC. Hence, ice volume plays a dominant role for LGM AMOC states, while the stability of interglacial AMOC states is dominated by atmospheric CO2. Therefore, the interplay of changes in ice volume and atmospheric CO2 determines the occurrence of bi-stable AMOC windows within the glacial-interglacial phase space. These findings, derived using COSMOS (ECHAM5/JSBACH/MPIOM), are currently tested in ongoing simulations with MPI-ESM and will be further tested with several different models including the AWI-CM within a concerted effort (lead by the PalMod member Dr. X. Zhang at AWI) as

part of PMIP4. Based on these developments, it is proposed to also produce simulations with AWI-CM for the next allocation period as outlined in the follow-up proposal.

Simulations with the AWI-CM studied the impact of fresh water flux from the GrIS. Accelerated melting due to global warming may significantly impact on the entire climate system. An estimate of freshwater (FW) flux from the GrIS is about 0.05 Sv from 1992-2010 and will increase (Bamber et al., 2012). The impact of FW flux from GrIS on climate is studied with AWI-CM for the Pre-Industrial (PI) based on 100 years of FW hosing (0.05 Sv, with spatial distribution along the Greenland coast) after 500 years of model spin-up. Mean strength of simulated AMOC for the unperturbed PI state amounts at 45°N to about 15 Sv. With FW flux due to GrIS melting, the AMOC drops by about 1-2 Sv (Fig. 3). Strongest decrease of AMOC during hosing occurs around 40°N and at a depth of about 1000 m.



Fig. 3: Simulated AMOC (100 yr) without and with GrIS freshwater hosing, and the anomaly.

The AWI glaciology group has incorporated a 3D ocean temperature component into PISM (v0.7.3) to improve the ice shelf basal mass balance in the model, that is one main driver of grounding line motion. Results for spin-up simulations have been submitted to the model intercomparison project ISMIP6/InitMIP-Ant. Numerous bugs in PISM (v0.7.3), especially in the bed-deformation part of the model, prohibit subsequent grid refinements. We therefore also implemented our methods in the current developer version of PISM. Unfortunately, this version still has serious problems with, for example, the reproducibility of model results. We

where therefore not able to perform the simulations ISM-1 (period 2017), prerequisite for ISM-2 and 3, until now. In addition, we are delayed by 3 months due to the parental leave of Dr. Thomas Kleiner (Jul-Sep. 2017).



The GFZ (PalMod 1-1-5 and 1-2-4) utilized VILMA to study sensitivity of earth structure and

**Fig. 4:** Simulated global rsl mean and standard deviation of model ensemble at LGM (21.5 ka) for a normal-distributed parameter space.

ice history on glacial isostatic adjustment and reconstructions of paleo-topography as a condition for the successful coupling of MPI-ESM with VILMA as well as for assessing sea level variability during the glacial cycle. For successful forward modeling of GIA during the last glacial cycle, the reconstruction of the initial topography was necessary. This data was determined by an iteration strategy. Results show that the iteration of paleo-topography converges fast and 4 iterations are sufficient. For the analysis of the paleo-topography and the effect of earth structure on GIA during the last glacial cycle, several model ensembles with different solid earth parametrizations were computed. Model ensembles with statistical assumptions of viscosity structure variability were calculated for different ranges of lithospheric thickness and viscosities of the upper and lower mantle. For example, results for a normal-distributed parameter space (lithospheric thickness [km]:  $\mu$ =103,  $\sigma$ =18; upper mantle viscosity [log<sub>10</sub> Pa s]: log<sub>10</sub>( $\mu$ )=20.7, log<sub>10</sub>( $\sigma$ )=0.2; lower mantle viscosity [log<sub>10</sub> Pa s]: log<sub>10</sub>( $\mu$ )=20.7, log<sub>10</sub>( $\sigma$ )=0.2; lower mantle viscosity [log<sub>10</sub> Pa s]: log<sub>10</sub>( $\mu$ )=22.2, log<sub>10</sub>( $\sigma$ )=0.3) show a relative sea level (rsl) variability of 73 m at the LGM, mainly confined to the former glaciation centers (Fig. 4).

Paleo-topography at the initial phase of a glacial cycle was analysed via model runs over two glacial cycles. Results indicate the need for implementing the previous glacial cycle before the last glacial cycle starts in order to provide a correct calculation of paleotopography at the initial phase of the last glacial cycle (Fig. 5).

To analyze the effect of ice-loading on the calculation of rsl and paleo-topography, different ice-history realizations found in literature were implemented. Models with loading histories from ICE5G (Peltier, 2004) and ICE6G (Peltier et al., 2015), as well as a combination from NAICE (Gowan et al. 2016) and ICE6G, were computed. These models were also calculated with different solid earth parametrizations.

Next to the sensitivity studies, the implemented restart options in VILMA, that were demanded for the coupling strategy followed at MPI-Met, are applied successfully (see above).



**Fig. 5**: Ensemble time evolution, rsl mean and standard deviation, over two glacial cycles at four locations, from the Laurentide ice sheet to the far-field.

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Project: **1030** Project title: **PalMod WG2** Project lead: **Victor Brovkin** Report period: **2017-01-01 to 2017-12-31** 

PalMod is a BMBF-funded project focused on understanding earth system dynamics and variability during the last glacial cycle. The PalMod project has a time scale of 4 years, with a potential extension up to 10 years. The first project phase will focus on the time from the Last Glacial Maximum to the present, while the second phase will consider the entire last glacial cycle.

WG2 of PalMod aims at understanding and quantifying feedbacks between biogeochemistry and climate during glacial cycles. Four work packages are focused on marine carbon cycle, terrestrial processes,  $CH_4$  cycle, and the dust cycle. Scientific challenges include reproducing the glacial  $CO_2$  cycle with comprehensive ESMs, understanding of rapid changes in atmospheric greenhouse gas concentrations during abrupt climate changes, and reconstructing atmospheric lifetime of  $CH_4$  using a coupled atmospheric chemistry model.

PalMod WG2 contains work packages WP2.1 "Marine carbon cycle", WP2.2 "Terrestrial carbon cycle", WP2.3 "Methane cycle", and WP2.4 "Dust cycle".

#### Reasons for not using all resources we asked for in 2017

- 1. Three of the subprojects were not able to use the computation time requested for 2017 as intended. WP 2.1 at MPI-M was strongly affected by personnel issues: The project postdoc left the group in late 2016 and it took a substantial amount of time to find a replacement, who is only now advanced far enough to be able to continue the work. Therefore WP 2.1 at MPI-M cannot report any progress for 2017 and used only very little of the computation time requested.
- 2. WP 2.1 at Universität Kiel asked for 54900 node hours of computing time on Mistral. 3900 node hours were planned to be used for stand-alone sensitivity simulations with MPIOM/HAMOCC to test and tune the ballasting parameterization with modern and LGM dust deposition rates. 51000 hours were planned to be used for two (one modern, one LGM) 2500-year-long time-slice experiments with the coupled, low resolution (T63GR15) atmosphere-ocean components of MPI-ESM. When the PalMod resources were cut by 42%, leaving us about 31800 node hours, it seemed impossible to still perform the coupled, T63GR15 simulations. Because we already knew from our experiments in 2016 that the uncertainties with respect to the particle ballasting parameterization were large, and that extensive parameter tuning was still necessary to achieve a more realistic biogeochemical state in the ocean, we decided to perform more uncoupled MPIOM/HAMOCC GR30 sensitivity and tuning simulations. To allow for the extra sensitivity simulations, and because we knew that the coupled, low-resolution simulations were no longer feasible, we planned to use the coarse-resolution (T31GR30) setup of MPI-ESM for our modern and LGM coupled atmosphere-ocean time slice experiments instead of the low-resolution

setup. However, since the LGM setup of MPI-ESM for PalMod has not been released yet, we have not started these coupled experiments. Rather than using (as initially planned) 3900 node hours for the ocean-only experiments, we have until now used about 18500 node hours for the uncoupled simulations. Since we, for the reason mentioned above, have not started any coupled time-slice experiments yet, we have to date only used about 60% of the approximately 31800 node hours that we were granted for 2017 (extrapolating our usage to the end of 2017, we will have used about 80 %).

3. WP 2.2 planned to re-calibrate the atmosphere model since it showed severe biases in surface-air-temperature, if the JSBACH permafrost code was enabled. However, further tests showed that the soil thermal dynamics are also not represented well in the model. Before this issue is improved, a re-calibration of ECHAM6 wouldn't make sense, it was therefore deferred until 2018.

# WP 2.1 "Marine carbon cycle", Universität Kiel

WP2.1 "Marine carbon cycle" aims at understanding and quantifying feedbacks between marine biogeochemistry and climate during glacial cycles. As part of WP2.1, TP3 focusses on the role that the acceleration of marine particles by ballast such as silicate and calcite minerals, and dust may have played for atmosphere pCO<sub>2</sub>-changes during the last glacial cycle.

To estimate potential changes of particle ballasting, in 2016 we had started to implement a new ballasting parameterization in MPIOM/HAMOCC. The inclusion of particle ballasting drastically affected particle sinking speeds in the model, which were previously prescribed at fixed values. This additional degree of freedom in the model required careful tuning of the ballasting parameters and also re-tuning of other HAMOCC model parameters, such as the remineralization rate of opal. This (re-)tuning of the ballasting parameterization and HAMOCC, as well as sensitivity runs with respect to reconstructed changes of the dust deposition rates, have been our focus in 2017.

In contrast to our 2016 estimate of the effect of enhanced dust deposition during the LGM on atmospheric  $pCO_2$ , we now allow for feedbacks of varying atmospheric  $pCO_2$  on atmosphere-ocean fluxes. That means, we diagnose the  $CO_2$ -flux-anomalies in each year, and update the atmospheric  $CO_2$  concentration accordingly in the following year, rather than assuming that the atmosphere is an infinite reservoir of  $CO_2$  at constant  $CO_2$  concentration.



**Fig. 1:** Simulated change of the atmospheric CO2 concentration in the control simulation (black, prescribed 278ppmv), compared to a simulation with LGM dust used only for ballasting while present-day dust is used for iron input (blue; CO2 change based on anomalous atmosphere-ocean fluxes relative to the control simulation), and to a simulation with LGM dust for both ballasting and iron (orange; assuming that 3.5% of the dust is iron, and that 1% of that iron is bioavailable).

With 1) a re-tuned (reduced by a factor of 6) opal remineralization rate, 2) the ballasting parameterization only applied below the euphotic zone, and 3) a flux-anomaly-based, interactive atmospheric  $pCO_2$ , our estimate of the effect of particle ballasting changes on atmospheric  $pCO_2$  is drastically reduced (Figure 1). According to our model, the contribution of particle ballasting by dust to the reconstructed LGM atmospheric  $pCO_2$ -drawdown by 80 ppm is only about 1 ppm or even negative, depending on the time scale (compared to our previous estimate in 2016 of 20 ppm within 200 years). The additional iron input associated with the enhanced dust deposition potentially caused over 20 ppm of the  $CO_2$ -drawdown according to our simulations, which is in line with previously published estimates of this effect ranging from 10 to 40 ppm.

To achieve 1) systematical uncertainty estimates with respect to the ballasting formulation, and 2) a quantification and understanding of the transient effects of ballasting changes during the deglaciation or even for the entire glacial cycle, traditional forward-integrations using MPIOM/HAMOCC will take too much time, even at coarse resolution. To still achieve these goals, we are planning to make use of the Transport Matrix Method (TMM) and the Marine Ecosystem Toolkit for Optimization and Simulation in 3-D (Metos3D) in collaboration with Thomas Slawig and Jaroslaw Piwonski (CAU Kiel) from PalMod WG4, who included a version of HAMOCC in Metos3D. First 3000-year-long simulations with Metos3D/HAMOCC on Mistral have shown that, using a coarse transport matrix based on a 2.8° MITgcm simulation (Khatiwala et al., 2005), the computation time can be reduced by a factor of 30 compared to the stand-alone MPIOM/HAMOCC coarse resolution setup.

#### WP2.2 "Terrestrial Carbon Cycle"

WP2.2 mainly planned to use computation time at DKRZ to re-calibrate the atmospheric model ECHAM6 to lessen the biases with regard to atmospheric temperature, if the JSBACH permafrost module was switched on. However, further tests of the permafrost module detected severe problems in thermal fluxes within the submodel, leading to thaw depths that are too deep for preindustrial climate and too shallow for LGM climate. The problem is illustrated in the following Figure. For preindustrial conditions, thaw depths for the northern Arctic should be between 30 and 50 cm, while they are more than 1 m in the model. While

thaw depths are unknown for the LGM, there are good reasons to believe they should be substantially deeper than the < 10cm modelled by JSBACH for large parts of the high latitudes. The cause of these problems has been identified, the problem is due to the fact that soil carbon, especially in the litter layer on top of the soil, is not properly accounted for in the thermal calculations. However, an update of the heat transfer scheme is still outstanding at this point in time.



Fig. 2: Thaw depth in JSBACH with permafrost for LGM (left) and preindustrial (right) conditions.

The result of this was that recalibration of the atmosphere model could not be performed as desired. The JSBACH permafrost module will have to be improved with regard to thermal dynamics before the recalibration of the atmosphere model can be attempted.



Fig. 3: Modelled vegetation carbon at LGM (left) and PI (right).

We also assessed the terrestrial carbon cycle for different climate states. The PI vegetation and carbon distribution (shown above) generally conforms to observations, while the LGM distribution is similar to available Palaeodata. The model therefore appears to be ready for transient experiments over the last glacial cycle.

# WP 2.3 "Methane cycle" (MPI-M)

In 2017 we performed extensive tests of the terrestrial methane emission model embedded in JSBACH. For this evaluation, we tested several distributions of wetlands and several uncertain parameters in the methane transport model to determine the settings that best reproduce present-day conditions as a basis for modelling past conditions. The model was validated against remote sensing datasets of wetland distributions and against methane fluxes from atmospheric inversions.



**Fig. 4:** Terrestrial methane emissions from wetlands from the CH4 emission model (left) and from an atmospheric inversion (right). Both the spatial distribution of modelled emissions and the magnitude of emissions agree very well.



**Fig. 4:** Latitudinal distribution of terrestrial methane emissions from wetlands from the  $CH_4$  emission model using different wetland data sets and model parameterisations, compared to atmospheric inversions (red). Only two sets of model results (Topmodel fix and Prigent var) show latitudinal distributions similar to inversions.

Latitudinal distribution of terrestrial methane emissions from wetlands from the  $CH_4$  emission model using different wetland data sets and model parameterisations, compared to atmospheric inversions (red). Only two sets of model results (Topmodel fix and Prigent var) show latitudinal distributions similar to inversions.

Using the experiments performed we were able to constrain wetland distributions and methane model parameters. The calibrated methane model is able to reproduce the overall magnitude and spatial distribution of wetland methane emissions inferred from atmospheric inversions. From this basis we will be able to provide *credible* model estimates of wetland methane emissions. Work on the CH<sub>4</sub> sink model in ECHAM (in collaboration with MPI-C, see paragraph below) is well advanced, though still requiring calibration.

#### WP 2.3 "Methane cycle" (MPI-C)

Within the project year 2017, we have conducted numerical experiments with a focus on the LGM atmosphere physicochemical state, its oxidative capacity and sinks/lifetime of atmospheric methane. From our knowledge on the present-day conditions, we know that

the tropospheric CH<sub>4</sub> lifetime ( $\tau_{CH4}$ ) is mostly determined by the abundance of its main reaction partner, the hydroxyl radical (OH). OH is an extremely reactive and therefore shortlived compound (estimated PD lifetime is ~1.5s in the troposphere), whose rapid recycling is determined by the abundance of water vapour, light, reactive carbon- (RC) and nitrogenbased (RN) compounds. The latter, in their various combinations, maintain conditions that support "buffering" of the OH concentrations and hence the oxidation capacity of the atmosphere in general (see details in [1]); many of them stem from the man-made emissions in the PD. However, what conditions should we reckon for the past? Tackling this cardinal problem, we pursued the following research questions:

- What are the emissions and typical abundances of the RC and RN compounds are expected the LGM, as suggested by the process-based AC-GCM model?
- What are the resulting OH abundance and  $CH_4$  lifetime, respectively? Is it similar to the PD and PI conditions?
- Can we identify compound(s) that by large determine the average tropospheric OH abundance, recycling and buffering?
- Is there a simplified quantification (e.g., a regression fit) available for predicting the global CH<sub>4</sub> lifetime value? If so, what is the relative contribution of each parameter to the total variation of  $\tau_{CH4}$ , and in which domain?
- Ultimately, can we make any conclusions about the stability of the atmospheric oxidative capacity in the past climates?

In order to investigate these research questions we simulated decadal CH<sub>4</sub> evolution using the 3D AC-GCM model EMAC [2] which includes kinetic chemistry submodel [3] with the state-of-the-art gas-phase oxidation chemistry mechanism (MOM, [1]). We have prepared the LGM setup of EMAC and further tuned it in order to reproduce the climate state corresponding to the reference CMPI5 simulation with MPI-ESM-P (MEP, lgm\_r1i1p1-P experiment, [4]) in the same resolution (T63L47, up to about 0.1 hPa or 80 km). The input data for the trace-gas emission submodels of EMAC were adjusted to correspond the simulated MEP vegetation and biomass burning patterns. For greater consistency, atmospheric dynamics in EMAC were relaxed ("nudged") towards the MEP output; this also allowed simulating biogenic RC and lightning RN emissions closely corresponding to MEP climate. In order to investigate the dependence of the resulting atmospheric chemistry state on the reactive-gas emission strengths, several sensitivity simulations were performed, where the emission factors for various compounds/processes were probed.

#### Results

We obtained LGM CH<sub>4</sub> lifetimes in the range of 9–11 years which is comparable to the PI/PD conditions. Such is the consequence of the primary dependence of the simulated OH abundances on the lightning NOx emissions (see **Error! Reference source not found.**, left); the latter are estimated to be of the comparable magnitude compared to the PD conditions (see below). Only in the Low-L simulation, where LNOx emissions were drastically reduced (by a factor of 5), the respective  $\tau_{CH4}$  value is subrationally increased (above 18 years); otherwise, atmospheric OH is well buffered by the RN present in the free troposphere.



**Fig. 5**: Left: Simulated LGM atmospheric CH4 lifetimes as a function of lightning NOx emission. Right: LGM vs. PD lightning NOx source change in EMAC (error bars: ±2σ inter-annual var.)

We find a low sensitivity of  $\tau_{CH4}$  to the climate driven changes in temperature ( $\Delta \tau_{CH4} = +0.5$  yrs at tropospheric mass-weighted  $\Delta T_{LGM-PD} = -3.1$ K). Contrary to that, an accurate empirical fit of the global average  $\tau_{CH4}$  value is possible in the form:

$$TC_{CH4,fit} = \mathbf{a} \cdot (LNx + \mathbf{fRN}_{S} \cdot RN_{S} + \mathbf{fRC}_{S} \cdot RC_{S})^{\mathbf{p}} \cdot [B/B_{0}]$$

where LNx, RNs and RCs denote lightning NO<sub>x</sub> and surface RN and RC annual emission fluxes in Tg(C|N)/yr for the LGM CH<sub>4</sub> atmospheric burden B vs. simulated reference burden  $B_0$  (1062 Tg(CH<sub>4</sub>)). Obtained values of fRN<sub>S</sub> = (12.6±3.0)% and fRC<sub>S</sub> = -(0.15±0.07)% denote the relative importance of the surface emissions of RN (via buffering) and RC (via reducing) in determining global OH abundance, respectively. The exponential kind of the fit (at a = 16.5±4.0 and  $p = -0.31\pm0.19$ ) adequately reflects the inverse proportionality between the NO<sub>x</sub>/OH emissions/abundances and CH<sub>4</sub> sink/lifetime. Because LNOx appears to be of primary importance for the tropospheric OH distribution, we have further simulated the changes to this term as predicted by five different LNOx parameterisations available in EMAC for PD and MEP climates (see Error! Reference source not found., right). It is important to note, that the most advanced parameterisations (Grewe et al. and Finney et al.) predict changes that lie within the inter-decadal variabilities simulated both for PD and LGM. The reason for that is that LNOx source shuts down during LGM in the NH higher latitudes due to ceased convective activity, however it becomes rebalanced over the increased continental area in the tropics, in particular over Oceania and Pacific West. Other parameterisations predict similar changes for the high latitudes but smaller effect on the LNOx emission in the tropics; we judge them as less realistic. Further work will be done on calibrating the LNOx source in EMAC and MEP (in the version being prepared for the transient simulations), also using newly available observational data for PD [5]. Ultimately, our preliminary results suggest that atmospheric oxidative capacity in LGM likely persisted at the levels comparable to those of PD, which has important implications for studying budgets and past records of atmospheric trace gases.

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**WP2.4 "Dust cycle"** is focused on the interactive simulations of dust sources and depositions during the last deglaciation. The interactive model of dust emission, transport, and deposition as a modulator of the radiative forcing will be an intrinsic part of ESM and EMICs simulations in WG1. In addition, biogeochemical role of dust as a forcing for marine biogeochemistry through Aeolian transport and deposition of micro-nutrients (iron) will be explored together with WP2.1.

#### Project objectives

The objective of the simulations is to optimize the dust production module with regard to its applicability for climate simulations and to review the representation of predominant dust source types. The individual tasks are: (1) Assessment and optimization of the dust production model in ECHAM6-HAM2 (global scale; simulations at DKRZ). (2) Sensitivity study: Simulations at different spatial and temporal resolutions, and configurations of the dust production module allowing for detailed assessment of the atmospheric dust life-cycle, feedbacks, interacting and impacting mechanism (e.g. wind speed distribution).

#### Work achieved until 2017-10-31

In order to ultimately aim for a computationally efficient dust module implemented in the ECHAM-HAM atmosphere-aerosol model, which is also the core of the MPI-ESM model, we are applying a two-stage approach:

Assessment of the current status of the ECHAM-HAM regarding computational cost of different model setups (T31L31-GR30 for 15 months): (a) ECHAM6 only (no dust or aerosol module called); (b) ECHAM6-HAM standard (full aerosol module called); (c) ECHAM6-HAM\_dust-only (only dust module loaded); (d) ECHAM6-HAM-JSBACH (dust sources limited by vegetation simulated by JSBACH).

ECHAM6	ECHAM6 with full HAM	ECHAM6 with dust- only HAM	ECHAM6 with dust- only HAM JSBACH based dust sources
7:41 min; 0.64 node hrs	20:44 min; 1.7 node hrs	13:30 min; 1.1 node hrs	14:15 min; 1.2 node hrs
6.2 min/year	16.5 min/year	10.8 min/year	11.4 min/year
1	2.66	1.75	1.84

For all simulations but simulation (a) dust was considered as passive tracer. Dust feedback on radiation and cloud microphysics was not considered this time.

Revisit of the dust module and feasibility study on reduced calling of dust routine and application of dust climatology (work still in progress, see figure below).



Fig. 6: Present-day dust emission and deposition.

ECHAM-HAM\_dust-only simulations were performed. Analysis of the results showed that regional tuning factors are required. These were introduced for present day dust emission for T31L31 with respect to T63L47 (Stanelle et al., 2014). Following extensive testing of the present-day setup, time slice simulations for LGM and Pre-Industrial (PI) were performed and analyzed.



Fig. 7: Ratio dust deposition LGM/PI.

#### References:

Stanelle, T., I. Bey, T. Raddatz, C. Reick, and I. Tegen (2014), Anthropogenically induced changes in twentieth century mineral dust burden and the associated impact on radiative forcing, J. Geophys. Res., doi:10.1002/2014JD022062.

# Project: **bu1029** Project title: **PalMod WG3** Project leader: **Andreas Hense, Ulrich Cubasch, Christoph Kottmeier, Martin Werner** Reporting period: **1.1.2017 - 31.12.2017**

# Report of works done on mistral from WG3.3 TP2 FUB

In WG-3.3 TP02 (FUB), the Data Assimilation (DA) of pseudo-proxies are successfully implemented and tested within an intermediate complexity model (SPEEDY) as well as the COSMO-CLM 5.00. The full results regarding the SPEEDY model is recently published (Acevedo et al., 2017, <u>https://doi.org/10.5194/cp-13-545-2017</u>). Therefore, here we report briefly on simulations using the COSMO-CLM model.

We assimilated the pseudo and real observations in CCLM model in three different sets of ensemble experiments: i) assimilation of pseudo-observations in an ensemble of 20 CCLM simulations (each of 10 years). ii) assimilation of pseudo-observations in an ensemble of 4 CCLM simulations (each of 36 years). iii ) assimilation of 500 E-OBS observations in an ensemble of 4 CCLM simulations (each of 36 years). The ensembles are generated by slightly shifting of domains from each other (1 to 5 grid points) and in 4 different directions (North-east, North-east, South-east, South-west). The proxy forward model used consists of nearest neighbour interpolation plus a random white noise with known standard deviation to create the pseudo-observations. The full results and the codes are under preparation in form of a paper entitled *"High Resolution Climate Reconstruction Using an Off-line Data Assimilation and COSMO-CLM 5.00 Model"* (the draft of the manuscript available here:

https://www.dropbox.com/s/3ucdxg3fj2s58w8/Manuscript\_Manu\_Walter\_Cubasch\_04.pd f?dl=0).

The comparison of COSMO-CLM model outputs and the pseudo-observations shows that the model seems to be well tuned for Central Europe. A region of significant model bias for both winter and summer seasons is located over the East side of the domain. This area is located far from the ocean where the ERAInterim data is prescribed (no coupled ocean was implemented). Therefore, we speculate that the model generates more variabilities and is free to evolve over this region. This biased behaviour is also observed in a real DA experiment using the E-OBS observation data set. Furthermore, we iterated the DA experiment on different values of correlation length for the summer and winter to find the optimal correlation length quantity. Afterwards, we showed that the skill of DA is linearly influenced by the SNRs used to create the noisy observations.



**Fig. 1:** 36-year unconstrained runs' (a and c for summer and winter) and analysis' (b and d for summer and winter) RMSE for seasonal mean of 2 meter temperature (K) with respect to E-OBS data. Red pluses show the locations of 500 selected observations from E-OBS.

Figure 1 shows the results of the assimilation of 500 E-OBS observations in COSMO-CLM simulations. Fig.1a and 1.c show the 36-year root mean square errors (RMSEs) of T2M for unconstrained simulations for summer (JJA) and winter(DJF). For comparison of model and gridded E-OBS dataset at 0.44°, the latter is bi-linearly remapped on the CCLM grid structure. The low model biases are located over East and North Europe: Germany, France, Spain, Portugal, Finland and United Kingdom for both winter and summer. In winter large biases are located over Switzerland, Italy, Morocco, Algeria and Russia. The RMSE values are generally larger in summer with high biases over South-east Europe and around Mediterranean Sea for example Bulgaria, Greece, Albania, Serbia and Ukraine. Figures 1.b and 1.d show that the model bias is largely reduced by assimilating 500 E-OBS observations. The importance of a homogeneous spatially distributed observation network is highlighted in these clips:

#### a) for winter : <u>https://www.dropbox.com/s/gma0gl9xgdnuxio/DJF.mp4?dl=0</u>

b) for summer: <u>https://www.dropbox.com/s/bj0z8lm10fr8c8m/JJA.mp4?dl=0</u>.

The number on South-West corner of the frame indicates the number of observations, which are assimilated. By increasing the number of assimilated observations to 2700 the RMSEs are largely reduced. This experiment shows that even a small number of stations (100) can contribute to a large error reduction in the analysis quantities. The distribution pattern of E-OBS stations in Central Europe is denser than East, West and South Europe. Therefore,

areas with coarse station population might require larger number of stations in order to achieve a homogeneous error reduction in the analysis.

### Simulations:

# SPEEDY-ENTKF

- 3  $\times$  24  $\times$  150 years of SPEEDY simulations with online DA (with initialization) with slab ocean and three different Proxy Forward Models (PFMs).

-  $3 \times 24 \times 150$  years of SPEEDY simulations with online DA (with initialization) with prescribed ocean and three different PFMs.

- 3  $\times$  24  $\times$  150 years of SPEEDY simulations with off-line DA (without initialization) with slab ocean and three different Proxy Forward Models (PFMs).

- 3  $\times$  24  $\times$ 150 years of SPEEDY simulations with off-line DA (without initialization) with prescribed ocean and three different PFMs.

# COSMO-CLM 5.00-EnsembleOI

- 21  $\times$  10 years of CCLM simulations with off-line DA.

# Report of works done on mistral from WG3.3 TP3 KIT

Various stable water  $[H_2^{18}O]/[H_2^{16}O]$  and  $[HD^{16}O]/[H_2^{16}O]$  isotope concentration ratios in precipitation are closely related to temperature and recorded in paleo archives such as ice cores and speleothems. To allow a quantitative and representative comparison of paleo simulations to these archives, KIT uses an isotope-enabled version of the regional model COSMO-CLM 4.8 (CCLMiso) (Pfahl et al. 2012).

For applying CCLMiso to the Arctic region, we added isotope physics at ice covered marine or continental surfaces to the model. For testing, debugging, and characterizing the new physics, we performed extensive simulation runs for the Arctic region (0.44°x0.44°, 159x176 grid points, 25000 node-h).

To validate the isotope-enabled CCLMiso simulations for the Arctic region, we performed a 15-year model run for present-day conditions as well as 10 sensitivity runs (0.44°x0.44°, 159x176 grid points, 40000 node-h). We found good agreement between the present-day simulation and observations of isotope ratios in precipitation and water vapor from the Arctic region (Global Network of Isotopes in Precipitation; remote sensing observations; campaign data from central Greenland). In addition, we found the accumulation-weighted annual isotopic composition of CCLMiso to be in good agreement with present-day snow pit samples. For this reason, CCLMiso simulations can be compared with ice core samples without accounting for biases.

Based on existing PMIP3 runs of the global isotope-enabled ECHAM5.4-wiso, we performed some preliminary simulations (0.44°x0.44°, 159x176 grid points, 10000 node-h) for the Last Glacial Maximum and a first model-data comparison with ice core samples corresponding to the LGM.



**Fig. 2:** Model-data comparison for water isotopes in present-day snow pit samples. Colored area: accumulation-weighted annual  $\delta^{18}$ O (normalized  $[H_2^{18}O]/[H_2^{16}O]$  ratio) in modeled precipitation; colored circles:  $\delta^{18}$ O of snow pit samples of (Weißbach et al. 2016).

#### References:

Pfahl, S., Wernli, H. & Yoshimura, K., 2012. The isotopic composition of precipitation from a winter storm - a case study with the limited-area model COSMOiso. Atmospheric Chemistry and Physics, 12(3), pp.1629-1648.

Weißbach, S. et al., 2016. Accumulation rate and stable oxygen isotope ratios of the ice cores from the North Greenland Traverse. 10.1594/PANGAEA.849161.

#### Report of works done on mistral from WG3.1 TP4 MIUB

PalMod is a BMBF funded project with the goal to simulate a full glacial cycle. For reference, proxy data such as plant pollen or ice cores are to assess the skill of the climate models. This working group focusses on the reconstruction methods based on proxy data as well as the uncertainties that are introduced by these means.

The earth system model MPI-ESM (version 1.2.00p4) is a state-of-the-art global climate model. In 2017, the atmospheric component ECHAM6 (version 6.3.02p4) has been used on HLRE-3 to generate an ensemble of simulations for the Mid Holocene (MH), approximately 6000 years before present. Sea surface temperatures (SST) and sea ice concentration (SIC) as boundary conditions were taken from a transient MPI-ESM simulation performed by Bader/Jungclaus. Furthermore greenhouse gases and orbital parameters have been set accordingly to past climate conditions. The model is coupled to the dynamical vegetation model JSBACH which e.g. describes interaction between plant functional types.

The ensemble consists of 13 members for 100 years each and was constructed by initializing the atmospheric model using restart files from the coupled run. The driving boundary conditions are transient and therefore physically consistent. For ten of the 13 simulations the atmospheric fields centered around 6000 years BP (namely at 6500, 6400, ..., 5600 years BP) were used with the corresponding transient oceanic boundary data. For these runs the used resolution in ECHAM6 is T63 with 47 vertical layers (L47) up to 0.01 hPa. The other three simulations are driven by the boundary conditions from 6100, 6000 and 5900 years BP with spectral resolution T63 as well but with a total of 95 vertical layers (L95). The increased number of layers allow for a better representation of the upper atmosphere compared to L47. It is expected that the thick scandinavian ice sheets during the LGM will affect the stratospheric dynamics which are known to influence tropospheric circulations. Hence, the L47 runs also serve as a reference for the L95 simulations that are yet to come.

All variables are written out by monthly means. Additionaly, the temperature in 2 meter height is given by daily means, which allows to calculate factors that more realistically represent the influence of plant growth and therefore improve the proxy-climate relationship.

Originally it was planned to perform additional simulations in 2017 for other time slices such as the LGM, approximately 21000 years BP, but due to unexpected unavailability of SST and SIC these runs have to be postponed to 2018. Nevertheless, the unused node hours were redistributed to another working group of PalMod. Also the MH study gave us several discernments about parallel computing as well as preprocessing the input data, setting up, testing and postprocessing climate models of high complexity. The practice of describing oceanic states was found to be not very successful in generating an ensemble in a sense that the resulting variances are much smaller, compared to those produced by multi-model ensembles such as the Paleo Model Intercomparison Project (PMIP).

However, using this ensemble it is possible to estimate important parameters that are needed in spatio-temporal climate reconstructions developed in the PalMod project. Examples of such variables are wind profiles, precipitation, temperature or albedo, some of which might not be available from PMIP. A major part in the paleo climate reconstruction process is the treatment of uncertainties. Therefore ensembles have to be generated to estimate covariance structures of e.g. temperature from the model runs.

A quick check whether ECHAM6 is able to simulate the different climate states is shown in the figure 3 below. The image on the left hand side shows the difference between the ensemble mean of temperature of coldest month (MTCO) and reanalysis ERA INTERIM as modern climate in Europe. In agreement with pollen proxy reconstructions Northern Europe experienced cooling in the Mid Holocene, even though the cooling is exaggerated. While Davis et al. (2003) reconstruct temperature anomalies around -1K, ECHAM6 models up to -3°C. Also Central Europe has temperatures comparable to modern values. The Sahara desert is modelled much colder as well. The plot on the right hand side shows the variance between the ensemble members of 20 year means of MTCO, which is the typical representative time scale of pollen reconstructions. It can be seen that in Northern Europe the largest variances geographically coincide with the overstated cooling.



**Fig. 3:** Temperature of the coldest month 100 year mean, ECHAM6 ensemble mean bias (left) relative to ERA-Interim Reanalysis, within Ensemble variance of mean temperature coldest month (right)

#### References

Davis, Basil AS, et al. "The temperature of Europe during the Holocene reconstructed from pollen data." Quaternary Science Reviews 22.15 (2003): 1701-1716.

#### Report of work done on mistral from WG3.1 TP1 HZG

For the report period 01.01.2017 - 31.12.2017 HZG did not use any computing resources from the PALMOD-BMBF Contingent bu1029. This relates to the fact that within Task 2.1 and Task 2.2 of WG 3.1, i.e. the HZG part, no numerical simulations have been envisaged, as the main part of the task of HZG is to establish statistical reconstruction techniques to estimate the non-climatic error in proxy time series. However, to test the robustness of those statistical methods the working group needs comprehensive numerical climate simulations in the context of pseudo proxy experiments. Therefor the HZG part of WG3.1 has a great interest in supporting those groups of WG 3.1 carrying out numerical simulations for the submission of a subsequent proposal for CPU time from the BMBF contingent.

#### Report of work done mistral from WG3.3 TP3 AWI

In 2017 the stable isotope algorithms have been implemented into MPI-ESM with resources taken from the AWI DKRZ shares. The model is ready for production simulation now.

# Project: **993** Project title: **PalMod WG4** Project lead: **Hendryk Bockelmann** Report period: **2017-01-01 to 2017-12-31**

#### Work Package 4.1

Up to now (October 2017), we have only performed some preliminary optimization runs with the HAMOCC model coupled to the Metos3D framework. These results are currently discussed with people from WG2. Thus we have (up to now!) only used a very small part of the planned computer resources. The main reason is that an operational optimization setting requires the coordination of different tasks: It consists of the driver which runs the actual optimization algorithm and the needed function evaluations. In this application, where a spin-up of the coupled transport-biogeochemical model is needed, the function evaluations themselves are very time-consuming and thus parallelized. As a consequence, run-time restrictions make it impossible to perform the overall optimization run "at once" as one process. The hardware restrictions (maximal run-time of processes) on the DKRZ HPC infrastructure are different from the one of our current local infrastructure in Kiel. Thus we had to restructure the organisation of interplay between main optimization processes and function evaluation processes. Moreover, in our current setting optimization is performed using Matlab or Octave, whereas the function evaluations are C/Fortran code. Since Matlab is not available for us on DKRZ, we had to alter the code to run with Octave.

These changes are now done, and we will perform more extensive optimization runs in the last weeks of this year. Thus, the total amount of consumed run-time in 2017 will come closer (than it is now) to the amount we applied for.

#### Work Package 4.2

State-of-the-art Earth System Models (ESMs) are not able to realistically simulate a glacial cycle because the orography and land-sea mask are fixed. We implement this capability into the Max Planck Institute Earth System Model (MPI-ESM) in order to be able of simulating the climate evolution during the last glacial cycle. Our goal is to automatically compute changes in the orography and land-sea mask throughout the simulation, while accounting for the conservation of mass and tracers. As such a condition, we propose the conservation not only on a global but also on a regional scale. Several experiments were performed to develop and optimise the desired time-varying land-sea mask for transient simulation. The runoff directions are calculated automatically as well as a function of the time varying topography allowing a redirection of rivers when the topography changes.

Regarding the CPU request for 2017 we performed the Ocean tests, the Ocean transient and some of the Coupled tests. For example, we run a test simulation with MPI-ESM and high-resolution topography prescribed from ICE-6G\_C reconstructions. The algorithms produce realistic features of the coastlines and river routing throughout time (Figure 1) while conserving mass and water properties. Nevertheless, we are still in a testing phase in order to improve the robustness of the algorithms and to guarantee a correct functioning under a wide range of bathymetry changes without introducing artefacts.



**Fig. 1:** Test simulation of the last deglaciation with an interactive land-sea mask, ocean bathymetry and river routing. Colors over ocean show the modelled sea surface temperature (SST; °C) and river discharge (m<sup>3</sup>s<sup>-1</sup>) over land.

# Work Package 4.3

We are up to now more involved in the pure technical coupling of different MPIESM/ECHAM resolutions than in performing extensive parallel-in-time computations with MPIESM. Moreover, we decided to additionally design a (technically) simpler experiment setting that can be run on local machines. The coupled MPIESM/ECHAM runs are postponed to the next year

# Work Package 4.4

The requested amount of node hours on GPU equipped compute nodes was not fully used in 2017 due to the strategic decision that porting parts of the ECHAM code to GPGPUs using OpenACC is no longer worth doing. The existing results on the CSCS Piz Daint supercomputer could not be verified on the DKRZ Mistral GPU nodes. Several shortcomings of the PGI compiler, that has to be used on Mistral for OpenACC enabled code, required a rewrite of too many parts since e.g. needed features are missing. Therefore, after the PalMod annual meeting in February 2017 no more compute resources on GPU partition were used.

Instead the implementation of the proposed functional/component-based parallelism approach was started in early 2017. Within this development phase the radiation module was extracted from the dynamics modules of the ECHAM code in order to run in parallel on dedicated MPI-tasks. A similar approach was also taken at MPI-M for the ICON model, such that a close collaboration and generic testing was indispensable. These steps required only small batch jobs to be run on Mistral and hence the requested amount of nodehours was currently not fully used.

At CAU Kiel a reduced/mixed precision implementation of parts of the ECHAM model should have been developed in 2017. Unfortunately, delays in personnel support forced us to postpone the work.