Dear Editor,

please find below the detailed answers to the referee comments including the resulting changes made to our revised manuscript, as already publicly uploaded as final author comment to the discussion of our manuscript. We additionally appended the latex-diff of the manuscript published by GMDD and the revised version.

Best regards, Astrid Kerkweg (also on behalf of all co-authors) Authors response to "Interactive comment on "The on-line coupled atmospheric chemistry model system MECO(n) - Part 5: Expanding the Multi-Model-Driver (MMD v2.0) for 2-way data exchange including data interpolation via GRID (v1.0)" by Astrid Kerkweg et al."

Note: Referee comments are indicated in bold, answers are in regular blue font.

Overview:

This manuscript documents new features of the MECO system (MESSyfied ECHAM and COSMO models nested). A new version (MMD v2.0) of the Multi-Model-Driver has been implemented and the capabilities of the 2-way coupling is illustrated. General Comments: a) The manuscript is well written and the achieved model improvements are clearly described. Thanks!

b) A description of the time management during the 2-way coupling is missed. I would see a more detailed explanation in terms of coupling frequency, time slices considered to average (accumulate) fields before interpolation, etc.

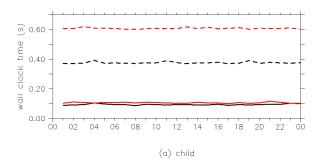
Usually people are aware of other couplings (e.g. ocean-atmosphere coupling) in which, for instance for mass conservation, fluxes need to be accumulated / averaged over the coupling interval. In contrast to this, our two-way coupling of two atmosphere models utilises a relaxation technique at the lateral boundaries for the parent-to-child exchange, and within the entire coupling domain for the feedback from child to parent, thus modifying the model results according to the finer resolved fields. Thus, since we do not couple fluxes for which mass conservation would be required, but correct the results directly, no accumulation or averaging is reasonable.

The coupling frequency can be changed per namelist, but to minimise the errors, it is strongly recommended to couple every parent model timestep. We add this information to the revised article within a newly added section "Model performance".

c) An evaluation of the MMD v2.0 model performances (the increased computational cost quantification, etc) compared to the v1.0 could improve substantially the present work.

Fig. 1 gives an impression of the costs of the coupling. A MECO(2) setup, similar to the hurricane case, was run for one day. During this simulation the wall clock time spent for the data transformation was measured using an internal tool utilising system clock counts. Because the child model does all the data transformations between the two grids, it consumes much more computing time than the parent model. The difference between the one-way coupled (black) and the only dynamically two-way coupled (red) simulation is small, as only six additional fields need to be transformed. Adding 139 chemical tracers to the one-way coupled setup (black dashed line) triples the processing time in the child model, while it requires the sixfold time, if they are two-way coupled (red dashed line). In contrast to this, the number of coupled fields provokes no systematic increase of computing time in the parent model.

We add this to the revised article in a new section "Model performance".



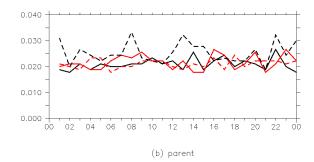


Figure 1: Hourly averaged wall clock time, spent for the processing of the coupling data in the submodels (a) MMD2WAY_CHILD and (b) MMD2WAY_PARENT for a MECO(2) setup, for different couplings between the two COSMO/MESSy instances: Black: Oneway coupling, red: two-way dynamical coupling. The dashed lines are for the additional coupling of 139 tracers.

Specific Comments:

- Page 3 line 5: I suggest to uniform the syntax and to use coupling OR nesting throughout the paper.

"Nesting" and "coupling" do not mean the same thing. The term "coupling" is much broader. In the context of model coupling, it describes the exchange of data between models (or components of those) in general. The term "nesting" is more specific. It describes the data transfer between two models of the same compartment (e.g. atmosphere), of which one typically resolves a larger domain and is used to drive the model with the smaller domain.

In order to explain the nature of our coupling correctly, we think, we need both terms in the abstract / introduction. In the remainder of the article (i.e. in two examples 4.2 and 4.3.2) we replaced the term "nested" by "on-line coupled" in order to unify the usage of nesting and coupling.

Page 5 line 25: what do you mean with "longer simulation"? I assume this system as also available for climate simulations, thus "restarting feature" is a mandatory requirement. Is it the system designed considering this feature? "Check-pointing", which is the technical term for "restarting feature", is indeed considered for the reasons given in the text. We remove "For longer simulations" and rewrite simply "Check-pointing" (the technical term for restarting feature) is required (not only for climate simulations) to be able ...".

Page 6 line 20: figure 3 labels (panel b) are not readable. Also please uniform the subpanel labelling [a), b) ..] in all of the manuscript figures. Labels are changed / updated.

Page 7 line 5: is there any plan to add other remapping approaches?

Yes. Especially, as SCRIP provides other horizontal remapping approaches, it is relatively straightforward to implement them as well. But there is no special need (and funding) to do so at the moment. Additionally, it is discussed whether to implement YAC (Hanke et al., GMD, 2016) into GRID.

Page 7 line 10: you use "0. and 1." Instead of the "1. and 2." Approach used in the previous page. Why?

Because the previous page gives just a list of steps which are processed, while here "0. and 1." are indeed the numbers, which can be set in the namelist to choose the "method". To avoid the confusion, we change the numbers on page 6 to bullet points and use quotes for the numbers on page 7.

Page 8 line 15: figure 4 labels are not readable. Changed.

Page 9 line 1: "as one central part" should be "as the central part"

This seems to be a misunderstanding due to incorrect use of language. Grid transformation is only one of a number of important parts in a model infrastructure. Others are e.g., memory management or time and event handling. Therefore we rephrase to "one important part".

Page 9 line 4: What does "ideally" means?

"Ideally" means that in the best case, the GRID submodel provides all the listed functionalities. So far, not all of them are implemented. This will be clarifed in the revised article.

Page 11 line 15: The remapping steps mentioned (first horiz. then vert.) are the typical ones. Not sure this is always the best way, depending on spatial resolution and fields considered. Is it possible to give the user the possibility to choose the interpolation order?

With some considerable additional programming effort it would be somehow possible. However, as usually the biggest problem is the height correction required due to the differently resolved orographies of the child and the parent model, it seems to be a natural choice to first regrid horizontally and to perform the vertical regridding intertwined with the height adjustment as a second step. At the time being we are not convinced that the effort of code restructuring would be justified by the scientific gain. We explicitly state this in the revised article.

Page 12 line 10: the last sentence of this chapter is a conclusion before results description. I suggest to move it after the discussion of the TC example.

Done.

Page 12 line 15: "For 2-way applications." please rephrase this sentence. We changed "For 2-way coupled applications the questions, if the aggregation of the subgrid-scale information provided by the smaller scale model to the larger scale model constitutes an added value for the larger scale model is still under debate." to "The question, if the aggregation of the subgrid-scale information provided by the smaller scale model to the larger scale model constitutes an added value for the larger scale model is still under debate and might be answered with the help of 2-way coupled applications."

Page 12 line 25: "NO" must be typed explicitly. Done.

Page 12 line 30: if I understand well, the only interpolation available is a conservative one. I suggest to add NO spatial integral values as obtained after and before the interpolation, to complement the information obtained by figure 5 and 6.

The NO emission flux integrated over the coupled domain is $3.29 \, kg(NO)/s$ and $2.63 \, kg(NO)/s$ for the parent and the child model, respectively. Thus, the differences in the soil properties of the two models account for a difference of $0.66 \, kg(NO)/s$. The integrated NO emission flux regridded from the child to the parent grid is $2.78 \, kg(NO)/s$, providing an emission flux lower by 0.51kg/s compared to the directly calculated integrated emission flux. The difference of $0.15 \, kg(NO)/s$ between the flux on the regional domain and its integral on the global domain simply results from the not fully congruent areas (due to different grid box sizes and orientation) over which the integrals are taken in the rotated domain and the global domain, respectively.

We add this information to the article.

Page 13 line 30: I think it could help to see in the present work also the model deficiency induced by topography.

Differently resolved topography heights in the coupled models cause a displacement of the tracer with height. To visualise these differences, a MECO(2) simulation with a passive tracer was performed. The initial tracer distribution is horizontally homogeneous and vertically increasing. Fig. 2 displays at four different locations, the height profiles of the tracer in the parent domain (black, triangles), in the child domain (blue, circles) and the coupled field (red, upside down triangles). The annotation gives the surface height in the parent and the child domain, respectively. The blue and the black line are always on top of each other indicating the tracer is initialised with exactly the same height profile in both COSMO instances. With increasing surface height difference, the difference in the vertical profiles increases. The second row of Fig. 2 displays the differences of the black and the red line, i.e., of the original profile and the profile given by the coupling field.

We will add this explanation to the supplement of the paper and add a reference to the supplement to the paper.

Page 14 line 10: what do you mean with "performed without any scaling of the emissions"?

Dust emission schemes heavily depend on soil properties, soil wetness and wind speed. All these factors vary with model resolution. Therefore, our dust emission scheme needs to be optimised by scaling the simulated flux for a given horizontal resolution, in order to yield the same integrated emitted dust mass. In this example we used the same scaling factors as for the global model in T42 also for the regional model.

We change the sentence to "without any resolution dependent optimisation of the emission scheme"

Page 15: are we looking (figures 10 and 11) at daily or 6hourly (or model time step snapshot) values? Is it possible to see the same as figure 10, but based on 10 meter wind speed?

These are 6 hourly values. We add this to the caption of the figure.

Fig. 3 shows the maximum 10m wind speed. As these figures do not provide any additional insights, we are hesitating to include them into the revised manuscript.

Page 15: I think it is really important to highlight the role of the coupling frequency when coupling components/models to improve the representation of certain features such as TCs (see Scoccimarro et al. 2017 and Zarzycki et al. 2016). Thus please add some comment on the coupling frequency you used and some information on sensitivity tests (if any).

Due to technical reasons, the frequency of data exchange between the child and the parent model must be the same as for the parent-to-child data transfer. For the latter, the two slices of the boundary fields, for which COSMO performs a linear time interpolation, are filled with the data of the actual time step of the parent model. This was required to enable the two-way coupling in which parent and child instances are running concurrently (and not sequentially). This approach enables an improved parallel scaling, but limits the (reasonable) choice of the coupling frequency. To minimise errors, the coupling frequency should be chosen as small as possible, i.e., the smallest common multiple of the parent and the child model time step. For this reason a sensitivity analysis of different coupling frequencies is not provided here. We add this information to the new section "Model Performance".

FIGURES: Figure 1 and 2 can be also smaller: I suggest to leave more space to enlarge figures as figure 4.

We reduce the figure size for the revised version. However, the production office might do different things.

Labels are not readable in figure 3a, 4, 10 and 11. Improved.

Please uniform subpanels labelling (also add it to figure 10 and 11. I suggest to set white colour for near 0 values in figures 3a, 4 and 9.

We added the subpanel labeling to Figs. 4, 7, 10 and 11.

We changed the color to white for near 0 values in Fig. 9 and to grey for Figs. 4 and 5 as the model domains should be distinguishable in the figures. However, for Fig. 3a there are no 0 values, as pink symbolises the EMAC domain.

Best regards, Astrid Kerkweg and co-authors

Literature:

Hanke, M., Redler, R., Holfeld, T., and Yastremsky, M.: YAC 1.2.0: new aspects for coupling software in Earth system modelling, Geosci. Model Dev., 9, 2755-2769, doi:10.5194/gmd-9-2755-2016, 2016.

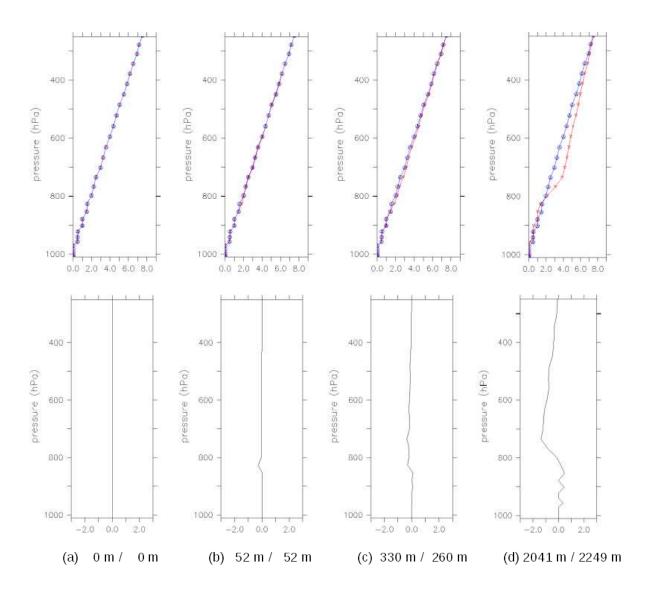


Figure 2: Vertical profiles of passive tracer (upper row) and their differences (lower row) for different topographic heights in the two COSMO/MESSy model instances (in $10^{-10} mol/mol$). The title gives the topographic height in the parent / child domain, respectively. Black line (triangles): initial profile in the parent model; blue line (circles): initial profile in the child model; red line (topdown triangles): coupled tracer profile in the parent model. The lower row displays the differences between the black and the red lines.

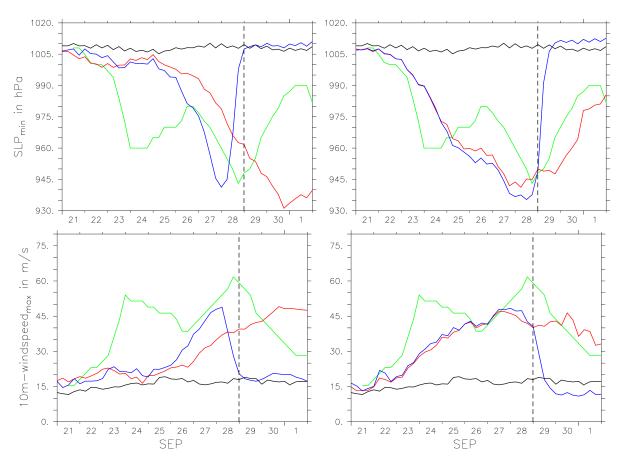


Figure 3: Time series of SLP_{min} (upper row) and 10 m wind speed (lower row) (in the area of $10^{\circ}N-50^{\circ}N$ and $65^{\circ}W-25^{\circ}W$) in the one-way (left) and 2-way (right) coupled simulation for EMAC (black), $COSMO/MESSy_{0.22^{\circ}}$ (red), $COSMO/MESSy_{0.11^{\circ}}$ (blue) based on 6-hourly data. The best-track intensity from HURDAT is shown as reference (green). EMAC is nuged until 29 September (dashed line, s. manuscript for details).

Authors response to "Interactive comment on "The on-line coupled atmospheric chemistry model system MECO(n) - Part 5: Expanding the Multi-Model-Driver (MMD v2.0) for 2-way data exchange including data interpolation via GRID (v1.0)" by Astrid Kerkweg et al."

<u>Note</u>: Referee comments are indicated in black and bold, answers are in regular blue font, and changes to the revised manuscript are highlighted in lightblue.

Dear Referee.

thanks for the careful reading of our manuscript and valuable hints on shortcomings in its original form.

R1: This manuscript is part 5 of the documentation of the MECO(n) online coupled atmospheric chemistry system. It presents an update of the Multi-Model-DriverMMD from v1.0 to v2.0, which introduces the option of 2-way (as opposed to 1-way) coupling, and describes a new submodel GRID v1.0 for grid translations between the coupled model systems. Online coupling of different model systems running on different grids, with different input and output requirements, different time steps, etc. and running as separate executables is a challenging task. The authors have done a marvelous job in accomplishing such a coupling between a global and a regional model and even between different instances of the regional model. The work is obviously not yet complete, and thus this publication should be seen as another update or extension. The manuscript is composed of a main part and comprehensive user manuals of MMD and GRID as supplements. The supplements provide all the details that are important for users. While I did not have time to look at them in detail, they seem to be well organized and comprehensive with detailed information on data structures and routines and the overall logic. The main body of the manuscript is a high-level description of MMD and GRID and, in addition, presents a few example applications of the coupled system. To me this looks like an appropriate approach for a GMD publication.

General/major points:

An important general question for a journal like GMD seems to me at what stage an update of a model deserves to be published. In my view only major updates that add significant new functionality should be published, and such updates should be in a mature stage. While the first criterion is clearly fulfilled by the present manuscript (a 2-way coupling is certainly a major update), the second point is much less clear, as detailed especially in point 1 of my main concerns below.

A1: We do not share the referees concern about publishing the system in the current state for several reasons: First of all, major parts of the described 2-way coupling, in particular for atmosheric chemistry related applications and diagnostics are technically complete and already in use. These applications deserve a proper reference, which can be cited if it comes to publications. Second, the current development step was released with the release 2.53 of our model system (see Section "Code

Availability") to a wider user community. This requires a proper reference and documentation, including a clear description of the current limitations.

- R2: Although the manuscript is reasonably well structured and written and the topic is relevant and suitable for GMD, I have some major reservations: 1. The 2-way coupling is still in a pre-mature stage
- A2: As above, we disagree. The 2-way coupling is technically complete and the updated model system is already in use, in particular for atmospheric chemistry related applications. These are in the focus of our work. Thus, we think, publication of the current stage of the developement is justified, despite the fact that the dynamical 2-way coupling, which is a specific challenge on its own, requires further development.
- R3: because a) dynamical 2-way coupling (of meteorology) seems not yet possible between EMAC and COSMO and even between instances of COSMO only seems to work reasonably well over flat terrain (an example is presented over the ocean). The main reason for this seems to be inconsistencies in the vertical grid transformations, especially because different methods are used for the partent-to-child (int2lm) and the child-to-parent (GRID v1.0) transformations.
- A3: This is correct for the EMAC-COSMO coupling. However, for the COSMO-COSMO coupling the vertical interpolation routine of INT2LM is used for both directions. We have to admit that this is not clear in the paper, but well documented in the supplement.

We add this information to the revised manuscript. The major problem for both, EMAC-COSMO and COSMO-COSMO couplings, is that INT2LM does not only perform a vertical remapping, but makes a crude assumption of keeping the boundary layer (i.e. up to 850 hPa) as it is, however, moving it to the height of the target orography and remapping only the remaining part of the vertical column. This procedure, as it is implemented in INT2LM, is not reversible and thus introduces spurious effects for different orographies, which are always present because of the different horizontal resolutions of the nested models.

- R4: b) as just mentioned, the COSMO pre-processor tool int2lm is still used for the parent-to-child transformations, which seems redundant since GRID should provide all functionality required for this, and using GRID for both up- and down-scaling would provide much more consistency. It remains unclear why this issue has not been resolved.
- A4: INT2LM provides much more functionalities than only remapping. It reads and processes the external data required as input for the COSMO model (especially for the initialisation of the model). Moreover, it performs some field adjustments concerning inconsistencies between the land-sea-mask of the COSMO model and the in-coming data.

We add this information to the introduction of Sect. 2.

Therefore, it is not possible to completely eliminate INT2LM. One could, however, indeed exchange the horizontal and vertical interpolation routines. We started to test this, but in the first place the performance (w.r.t. the results) of the child model was downgraded. As explained above, the main problem is the extra treatment of the boundary layer, which for the off-line nested COSMO model is the preferred way, as this makes physically more sense compared to a simple vertical

interpolation. But in terms of reversibility of the height adjustment procedure this unfortunately causes problems.

- R5: c) The GRID submodel seems to be still in a fairly rudimentary stage. E.g. only "conservative remapping" is implemented (see P7, L6), whereas the description of the GRID submodel in Section 3 also mentions "interpolation" as a final goal (see P9, L15). Also vertical grid transformations seem to be implemented only in a pre-mature way (see next point).
- A5: This is obviously a misunderstanding that we need to clarify. Please do not mix up GRID with the applied interpolation procedure for the 2-way coupling in MMD2WAY. GRID is fully functional, it includes two remapping packages: NREGRID and SCRIP, implying that all interpolation / remapping routines provided by NREGRID and SCRIP can be used with the GRID submodel.

For the 2-way coupling (MMD2WAY), however, only conservative remapping is utilized so far, for mainly two reasons: First, an improved run-time performance can be achieved by efficiently exploiting the given horizonal domain decompositions of the models, because the data exchange between the local domains could be minimised in comparison to other remapping or interpolation schemes. And second, conservative remapping is the first choice for atmospheric chemistry applications, since fluxes (e.g. emission fluxes) are conserved.

We are more precise about this in the revised manuscript.

We change the sentence on page 7 from "For the time being, only conservative remapping is implemented as horizontal transformation method" to "For the time being, only the conservative remapping, as provided by GRID, is utilized as transformation method in MMD2WAY_CHILD."

- R6: Some parts of the manuscript are lacking clarity and detail. I am particularly missing details regarding the grid transformations and the separation into horizontal and vertical transformations. In particular, COSMO is a non-hydrostatic model running on a geometrically fixed grid, whereas EMAC is hydrostatic and formulated on a hybrid-pressure grid. Although I understand the motivation of the authors to keep the descriptions generic, the transformation between these fundamentally different vertical representations is essential and should be much better described.
- A6: The revised manuscript contains a more detailed description.
- R7: Furthermore, COSMO variables are represented on a staggered (Arakawa-C type) grid, which requires different transformations for variables like temperature or concentrations defined on grid cell centers, and variables like wind or tendencies defined on grid cell interfaces. Neither the main body of the manuscript nor the documentation makes any reference to the issue of staggered variables.
- A7: The only variables defined on the staggered grid in the COSMO model are the wind components. For the COSMO-EMAC coupling the COSMO wind components are first interpolated to the cell midpoints, and afterwards transformed to the EMAC grid. For the COSMO-COSMO coupling the wind components are interpolated directly between the staggered grids, i.e., they are always defined on the box edges. This information is added to the revised manuscript and the MMD User Manual.
- R8: The manuscript talks about a "geo-hybrid-grid" without explaining this structure [...]

A8: The Fortran data structures of GRID are based on those of NCREGRID as published by [Jöckel(2006)]. This article provides an extensive explanation of the definition of a geo-hybrid grid. Therefore, we did not repeat it in the current article. [Jöckel(2006)] introduces the geo-hybrid grid as follows: The horizontal grid space of a geo-hybrid grid usually comprises geographical latitude and longitude. Especially in 3-D global atmospheric models the vertical pressure (p) coordinate is often defined by hybrid levels (with index i) of the form

$$p(i, x, y, t) = h_a(i) \cdot p_0 + h_b(i) \cdot p_s(x, y, t), \tag{1}$$

where p_s is the surface pressure, p_0 is a constant reference pressure, and h_a and h_b are the dimensionless hybrid coefficients. This representation in a curvi-linear coordinate system (dependent on longitude x, latitude y, and time t) allows a terrain following vertical coordinate, if $h_a = 0$ and $h_b = 1$ for the lowest level (surface level)."

Thus, dependent on the choice of p_s and p_0 GRID is capable to handle all cases of vertical pressure axes, such as

- hybrid pressure axes $(h_a \neq 0, h_b \neq 0)$,
- constant pressure axes $(h_b = 0)$ and
- sigma levels $(h_a = 0)$.

In the case of $h_b = 0$, $h_a \cdot p_0$ could also be a height coordinate. The grid transformations require that source and destination grids are both defined in the same vertical representation, i.e. either with pressure or with height coordinates.

We add some more information to the revised Sect. 3.1 (which also required a slight reordering), with a specific reference to the corresponding section in the revised GRID User Manual, which contains the complete information.

- R9: [...] and later about the "basegrid".
- A9: "basegrid" is a short cut for one specific geo-hybgrid grid, namely the 3-D grid of the basemodel (see Sect. 3.2 in the GMDD version of the manuscript).
- R10: GRID seems to expect a hybrid pressure grid (see line 14 on page 10), but how COSMO variables are transformed to hybrid pressure levels is never explained.
- A10: The COSMO model still provides the possibility to define the vertical grid by pressure levels. This option was still frequently used when our model development started. Thus, for the definition of the hybrid pressure grid, we currently use the routines provided by INT2LM.

Nevertheless, in the meantime GRID is further developed to deal with the requirements of the ICON model, which only features height axes. Thus, we are going to implement the possibility to use the actual (time-dependent) 3-D pressure field for remapping between height and pressure grids, since this will be required for the MESSy infrastructure submodel IMPORT connected to ICON.

We discuss this issue more in the revised Sect. 2.2.

R11: Furthermore, if GRID only supports hybrid-pressure levels, it will be little suited for transformations between two instances of COSMO, as these are both operating on geometric grids.

- A11: As explained in answer A8, height height interpolations are possible as well. Anyhow, as stated in answer A3, for the back-transition between two COSMO instances the procedure of INT2LM is used.
- R12: I am also missing information on details of the coupling, especially with respect to the frequency of the coupling: Are fields exchanged at every model time step? Are the parent and child models forced to use the same time steps? Is the frequency of coupling the same for the upward and the downward directions? Such information my be added in Section 2.2. 3.
- A12: Parent and child model do not need to use the same time step lengths. However, the parent model time step length needs to be a common multiple of the child model time step length. The coupling frequency can be changed in the namelist, but to minimise the deviation of the child model from the parent model state at the boundary, it is strongly recommended to couple every parent model timestep. This information is provided in a new subsection "Model performance" of the revised manuscript.
- R13: The authors emphasize the need for developing computationally efficient interfaces and submodels (e.g. line 19 on page 9), but no information is provided that would allow the reader to judge the efficiency of the coupling that is ultimately achieved. What is the computational overhead introduced by the coupling in terms of additional memory usage and computation time? Maybe this has been addressed in previous publications, but if so, this should be referenced. Otherwise, I would strongly encourage the authors to benchmark the model system (e.g. for one of the simulation examples in Sect. 4) with detailed timings of the individual model components and additional diagnostics, as this is a fundamental first step towards identifying bottlenecks and improving efficiency.
- A13: It is not clear to us, to which reference this "overhead" and additional computation time should be compared to? An off-line 2-way nesting is hardly possible, and the show-stopper would obviously be the tremendous I/O required to write and read the files with coupled fields in every model time step. The required memory (for the 2-way nesting) increases linearly with the number of variables that need to be exchanged. And the run-time performance depends first and foremost on the specific model setups (e.g., on the complexity of the chosen chemistry representation etc.). But most important, the overall performance is at the end determined by the "degree of balance" of the distribution of parallel tasks among the different model instances. We discussed this in detail in Part II of our series (Kerkweg and Jöckel, 2012) for the 1-way nesting case. The same principles hold for the 2-way exchange, except for the complication that communication waiting times depend now on bidirectional data exchange. Thus, it is up to the user to find (experimentally) the optimum task distribution to minimise communication waiting times.

We add a brief discussion on this to the new Section "Model performance" and additionally assess the dependency of the simulation time on the number of coupled fields in order to check, whether an increasing number of fields shows discontinuously prolonged simulation times caused by the 2-way exchange.

R14: The manuscript may be acceptable after addressing my main concerns 2 and 3 (plus the minor points below), or it may be postponed until a

more mature version of coupling is available (i.e. main concern 1 is also addressed).

A14: See our answers A1 and A2.

R15: Minor points: - Introduction: The reasons for the external coupling mentioned on P2/L20-30 are not entirely clear. Why is it good to "prevent the patches approach"? What are the "limitations of the Fortran95 namespace"?

A15: Maybe we were not precise enough here. The "patches approach" is usually a feature of regional grid-refinements, which is directly embedded in (or part of) the model code, as for instance in WRF or ICON, in which the user can specify the number of patches and their corresponding domains flexibly at run-time. For such a feature, however, the entire model code needs to be "aware" of a(n arbitrary) number of grid-refined patches. Thus, this needs to be implemented "by design". To equip legacy code (as COSMO or ECHAM) supplementarily with such a feature would basically mean to rewrite the entire code from scratch. The reason is that all prognostic (and diagnostic) variables need to exist on each patch (technically independent of each other). How this is technically achieved depends largely on the applied programming language. In fully object oriented languages, overloaded "sets" or "instances" of the same variable(s) could be defined, however, the Fortran95 language standard does not allow to have the same variable with the same name in the same name-space more than once. Thus a complete recoding, e.g., replacing arrays by structures of arrays is required.

The first /second part of this answer is added for clarification to the first / second bullet point in the introduction of the revised manuscript.

R16: On the other hand, an advantage not mentioned is that this external coupling allows testing the influence of the coupling of different (individual) variables, which would likely be more difficult with internal coupling. The introduction should also emphasize the disadvantages and challenges of the external coupling, e.g. the challenge of transforming between different vertical grids.

A16: First of all, thank you very much for this important hint on variable testing. We add this point to our revised list of advantages.

Indeed, in our current applications we do exactly this (e.g., chemical 2-way nesting with dynamical 1-way nesting).

Concering the challenges: The need to transform between different vertical grids is not necessarily connected to the way of (internal or external) coupling. Nevertheless, the patch (or grid-refinement) approaches are usually implemented as "internal" coupling and do keep the vertical grid between different patches in order to avoid vertical interpolation. But also in an external coupling approach the vertical grid between different model instances can be the same. In both cases, however, the issues due to the horizontally refined orography information remain.

To expand the discussion, we add some statements about the disadvantages and challenges of external coupling to the revised introduction, right after the list of reasons for choosing external coupling:

"Apart from these advantages, the external coupling proves to be more challenging than the internal coupling. Horizontal and vertical interpolation errors are expected to be larger, depending on the relations between the different grids and differences in the orography. From these, the adaption to the higher resolved orography of

- the nested simulation causes the largest error. An additional disadvantage of all external coupling approaches is the need for the user to optimise the distribution of the available parallel tasks among the different model instances, in order to achieve an optimal run-time performance with minimized waiting times between the model instances."
- R17: Footnote "2" on MPI-ESM seems little relevant in the context of this manuscript and could easily be deleted in my view.
- A17: We want to provide references for each model.

 Instead of the web-site, we now cite Giorgetta et al. (2013).
- R18: **P3**, **L8**: Sentence "This article documents the development of the . . .". No, this article is only part of a documentation.
- A18: We change the statement to "This article documents a major achievement in the development of the ... "
- R19: The following lines are presented in italics, which I found confusing until I realized that this is a citation. It would be clearer to present the references at the beginning and then the quoted text, e.g. "As described in Jöckel et al. (2015), Baumgaertner et al. (2016) and the MESSy homepage (..), the Modular Earth System Model (MESSy) is "a sofware providing . . .".
- A19: Thanks for this suggestion! Indeed, the reordering enhances the readability a lot. Changed.
- R20: P4, L3: Delete the bracket "(Messyfied ECHAM . . .)", this was already explained earlier.
- A20: Done.
- R21: P4, L14: "update of MMD" \rightarrow "update of MMD presented here"
- A21: Changed.
- R22: At the end of the introduction section I was wondering whether GRID is now used for both directions replacing INT2LM entirely or not. It should already be explained here that the present implementation of GRID is only used for the child-to-parent transformation.
- A22: We change the sentence "Sect. 3 introduces the newly developed GRID submodel, which provides the required mapping functionalities" to "Sect. 3 introduces the newly developed GRID submodel, which provides the required mapping functionalities used for the child-to-parent data exchange.". Furthermore, the last sentence of the prior paragraph reads now "GRID can be used for all grid mapping operations required during a simulation." instead of "GRID is used for all grid mapping operations required during a simulation."
- R23: P6, L15: What does "imprints its time settings" mean? Start and end of the simulation, time step, or something else?
- A23: These are the start-date (only if a model instance is newly started), the end-date, and the restart trigger.
 - Item changed to "the parent imprints its time settings on the child model, i.e., end-date, restart trigger and, at the very first start of a model instance, the (re-)start-date as start-date of this instance."

- R24: Does "imprint" mean that the child model has to use the same time step as the parent?
- A24: No. Forcing the coarsest instance to use the same short time step length as the finest resolved model instance would downgrade the performance of the system dramatically. Nevertheless, the time step lengths of all model instances need to be common multiples.
 - For respective changes in manuscript: see A12.
- R25: P6, footnote 9: It would be better to include this information in the main text rather than as a footnote. Is it really necessary to distinguish between INT2LM and INT2COSMO in this manuscript?
- A25: We prefer to keep the differentiation between INT2LM and INT2COSMO to keep the manuscript consistent with Part II of the article series about MECO(n). We inline the footnote in the revised manuscript. The sentence reads: "Afterwards the data is transformed from the in-grid to the child grid using the expanded version of the preprocessing software INT2LM for the COSMO model (INT2COSMO). See Kerkweg and Jöckel (2012b) for further explanations."
- R26: P7, L9-16: What is the difference between Option "0" and Option "1a"? On line 16, shouldn't it be Option "0" rather than "(a)", since (a) was introduced as an option available only for prognostic variables?
- A26: With option "0", as explained in the text, the memory for the target field is allocated within MMD2WAY_PARENT and can afterwards be accessed by other MESSy submodels. For option "1", however, the variable needs to exist in the parent model and will be modified directly.

 In the revision, we change the wording from "the field is used to modify an existing parent model field." to "the exchanged field is used to directly modify a parent model field." Additionally, as the explanations below belong all to option "1", we moved the end of the enumeration to the end of the section.
- R27: P8, L17: The weight functions should remain the same during the simulation, at least the horizontal weights. Are the functions nevertheless transformed at each time step, i.e. the same transformation is repeated over and over again?
- A27: Indeed, our sentence is misleading. We change it to:

 "They are once, during the initialization phase, transformed in the same way as the data and sent to the parent model for application during the integration phase."
- R28: P8, L28: The statement "for all required grid transformations" is not correct, since int2lm is used for partent-to-child transformations.
- A28: This needs indeed to be clarified. GRID is independent of MMD2WAY. The MESSy infrastructure component GRID provides the basis for all required grid transformations. However, in the MMD2WAY_CHILD submodel we decided to use the INT2LM software instead of GRID. One of the reasons is that the 1-way online coupling was implemented prior to GRID.

 This sentence is skipped in the revised manuscript anyhow, see A29.
- R29: P8, L29: I didn't understand this sentence. "Ideally" points at an ideal state not yet reached and should therefore be followed by "would be implemented" rather than "is implemented".

A29: Yes. "Ideally" means that in the best case, the GRID submodel provides all the listed functionalities. So far, not all of them are implemented. This is clarified in the revised article. We change "is" to "would be".

Moreover, we see that the first sentence of this subsection is misleading. Therefore we skip it and add a more general introduction, fitting better the following more general statements. The new sentence reads: "Due to the increasing complexity of Earth System Models, grid transformations at run-time of the model, (e.g., remapping from an atmosphere grid to a higher resolved land grid and vice versa) are more and more commonly required. To avoid individual implementations throughout the code, such an on-line transformation functionality should be implemented as one important part of the model infrastructure, providing a common grid processing functionality."

R30: **P9**, **L1**: What exactly do you mean by "as one central part of the model infrastructure"?

- A30: This seems to be a misunderstanding due to incorrect use of language. Grid transformation is only one of a number of important parts in a model infrastructure. Others are, for instance, memory management or time and event handling. Therefore we rephrase to "one important part".
- R31: P9, L5-8: I don't agree with the definition of regular and irregular grids. A "lambert conformal" grid as often used e.g. in WRF is also a regular orthogonal grid. A grid is usually regular in one projection but irregular (non-orthogonal) in another projection. Here it sounds like any non-latlon grid would be irregular (same issue in Section 3.1).
- A31: Indeed, it was definitely not our intention to name every non-lat-lon grid irregular! Following the grid classifications of Bowler and Clegg (2011), we decided to change the grid classification to
 - rectangular grids, which are either orthogonal in geo-coordinates (rectilinear grids) or curvi-linear grids,
 - non-rectangular structured grids, and
 - unstructured grids.

The second sentence of Sect. 3.1 is changed accordingly to "Four different grid types are distinguishable: (1) rectangular grids, which are orthogonal in geo-coordinates, (2) curvi-linear grids, (3) non-rectangular, structured grids and (4) unstructured or irregularly geo-located grids.

- R32: Equally important as the horizontal grid transformation (and actually more challenging) is the vertical transformation. This needs more attention in section 3.
- A32: We provide additional information on the vertical remapping in revised Sect. 3. by introducing a new subsection "3.1.4 Application of GRID in MMD2WAY_CHILD".
- R33: P10, L11: What is a "geo-hybrid grid" structure?
- A33: A geo-hybrid grid structure is the Fortran type definition (= structure), which contains all data required to define a geo-hybrid grid (for the definition of a geo-hybrid grid see answer A8.)
 - We change the sentence to "The definition of the Fortran structure, which contains

- all components required for the definition of a geo-hybrid grid, was extended and generalised for the usage in GRID."
- R34: P10, L13: Why is a grid "defined by geographical longitude and latitude and vertically by hybrid pressure coefficients"? Is this a design choice for the GRID submodel?
- A34: Yes it is. See answer A8.
- R35: Does that imply that for a COSMO-COSMO nesting the COSMO grids (which may share the same projection) have to be first converted to geographical coordinates and then back to rotated ones? It would seem much more logical to me that GRID would translate everything to the same projection (e.g. the one used in the parent model), irrespective of whether it is a geographical coordinate system or not.
- A35: The referee comments R35, R37 and R39 point to an additional misunderstanding: In our article the term "grid transformations" refers always to data "remapping", "regridding" or interpolation between different model grids based on geographical coordinates. We never intended to use it in the meaning of "grid translations" or "map projection".
 - Independent of the computational grid of the model, the grid structure in GRID contains the data of the grid vertices and / or cell centers always in geographical coordinates. This information is in all cases provided by the respective base-models (ECHAM5 and COSMO) and does not need to be determined by the GRID submodel. Thus, GRID does not need to perform "grid translations" or "map projections". The remapping weights of geo-located data between two different grids are always calculated in geographical coordinates.
 - We change the term transformation to remapping at some location in the article to avoid the above misunderstanding. Additionally, the information about the geographical coordinates is added to the revised Sect. 3.1.
- R36: How is the COSMO vertical grid transformed to hybrid pressures?
- A36: Until now, the hybrid pressure coefficients calculated by INT2LM or the COSMO model are used. See answer A10.
- R37: Section 3.1.1 GRID_TRAFO: Grid transformations have been implemented in standard libraries like gdal (http://www.gdal.org/) and proj.4 (http://proj4.org), which also support rotated grids as used in COSMO. Why did you not choose to link to such a library that could provide a great level of flexibility? The SCRIP software seems to offer comparatively little flexibility. In my view one should strictly distinguish between coordinate translations (as can be accomplished by such libraries) and the final mapping between grids, which can be done by linear, cubic, or spline interpolation of any other (possibly conservative) mapping, and may be implemented as separate routines in GRID.
- A37: As far as we understand the functionalities of these libraries, they would not help, as it is not coordinate translations (or map projections) we need, but the actual remapping of data between different geographical coordinate systems.
- R38: Please make clear from the beginning that NREGRID is only implemented in GRID for vertical transformation, while SCRIP is used for

all horizontal transformations, not only at the end of Section 3.1.3 (and more explicitly in the conclusions). Otherwise the reader - like myself - is confused about the role of NREGRID.

A38: Sorry! Obviously we have to be more clear about the separation of GRID and the MMD submodels. NREGRID was originally implemented for horizontal and 3-D spatial remapping. This is still the standard way for the data import in the EMAC model (i.e., with ECHAM5 as basemodel).

In the COSMO model, some of the requirements of NREGRID w.r.t. the grid structure are, however, not fullfilled. Therefore, we had to introduce a second remapping option for horizontal grids, which can deal with rotated grids, such as the COSMO grid. We decided to use the very well known and commonly used SCRIP software package.

Therefore, MMD2WAY_CHILD uses SCRIP for the horizontal interpolations, and NREGRID for the vertical remapping, as SCRIP does not provide remapping along the vertical axis.

- R39: P11, L1: Why is NREGRID recursive? Is this information relevant here? It sounds strange to me to have a recursive algorithm for grid translations.
- A39: NREGRID is not for grid translations. It is for the rediscretisation of "gridded" geo-scientific data between n-dimensional (usually n = 2 or 3) orthogonal grids. The conservative rediscretisation of extensive or intensive variables is based on the calculation of the overlap (area or volume) matrix between source and destination grid boxes. For orthogonal grids these overlap matrices can nicely be calculated recursively, since the overlap area / volume is zero as soon as at least the overlap interval along one axis (dimension) is zero. For details see Jöckel (2006). Since the recursive nature of this algorithm limits its application to orthogonal grids it cannot be applied for rediscretisations between the (in geographical coordinates) orthogonal Gaussian grid of ECHAM5 and the rotated (in geographical coordinates non-orthogonal) COSMO grid. This is why we needed to implement SCRIP as well. Thus, the information is relevant.

We add this information to Sect. 3.1.2.

as atmospheric chemistry is highly non-linear."

els.

- R40: P12, L16: "For 2-way applications" \rightarrow "For 2-way coupling applications" A40: Changed.
- R41: P12, L21-26: A missing important point why size matters in atmospheric chemistry is that this chemistry is highly non-linear.
- A41: This is indeed what we meant.

 We rephrase the last sentence to "Especially in highly polluted regions, or more generally near emission sources, this might influence the simulated chemical regime,
- R42: P13, L7: dry deposition velocities do not only depend on soil type but also on turbulence, which could be another difference between the mod-
- A42: Thanks for this remark.

 We change the last sentence from ", which is most propably due to different soil properties in that region." to ", which is most propably due to different soil properties and also due to the different turbulence schemes employed by the two basemodels. "

R43: P15, L8: Is really only the pressure perturbation exchanged, i.e. the deviation from a reference pressure profile?

A43: For the COSMO-COSMO coupling only the deviation of the pressure from the reference atmosphere is exchanged during the integration. During the model initialisation phase all information required for the definition of the parent grid are exchanged. The definition of the reference atmosphere itself is part of this onetime data exchange. The term "pressure perturbation" seems to lead to a misunder-standing.

Therefore we change "pressure perturbation (pp)" by "the pressure deviation from the reference atmosphere (PP)".

Typos and grammar:

- P4, L30; "software as" \rightarrow "software such as"

Corrected.

P5, L5: "reasonable" seems not the right word here.

"This is reasonable," is replaced by "This was required,"

P7, L6: "At the time being" \rightarrow "For the time being"

Corrected.

P7, L17: "For both option" \rightarrow "For both options"

Corrected.

P12, L4: "handy" is not a good word in a scientific publication

Replaced by "useful".

P12, L6: "tools, can" \rightarrow "tools can"

Corrected.

P12, L31-32: Change to "If COSMO/Messy were 2-way coupled into EMAC and EMAC were using the NO emissions .."

Corrected.

P13, L2: "what is mostly" \rightarrow "which is mostly"

Corrected.

P13, L5: "pervious" \rightarrow "previous"

Corrected.

P13, L6: I would say "slightly but systematically" rather than "systematically"

Done.

P14, L4: "good" \rightarrow "well"

Corrected

P23, Fig. 5: "been mask" \rightarrow "been masked"

Corrected.

Best regards,

Astrid Kerkweg and co-authors

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The on-line coupled atmospheric chemistry model system MECO(n) – Part 5: Expanding the Multi-Model-Driver (MMD v2.0) for 2-way data exchange including data interpolation via GRID (v1.0)

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Abstract. This article is part of the model documentation of the MECO(n) system (MESSyfied ECHAM and COSMO models nested n-times). As part of the Modular Earth Submodel System (MESSy) the Multi-Model-Driver (MMD v1.0) was developed to couple on-line regional model instances into a driving model (see Part 2 of the model documentation). MMD comprises the message passing infrastructure required for the parallel execution (multiple program multiple data, MPMD) of different models and the communication of the individual model instances, i.e. between the driving and the driven models. Initially the MMD library was developed for a 1-way coupling between the global chemistry climate model EMAC and an arbitrary number of (optionally cascaded) instances of the regional chemistry climate model COSMO/MESSy. Thus MMD (v1.0) provided only functions for unidirectional data transfer, i.e., from the larger scale to the smaler scale models.

Soon, extended applications requiring data transfer from the small-scale model back to the larger scale model became of interest: e.g., the original fields in the larger scale model can directly be compared to the up-scaled small-scale fields to analyse the gain by the original small-scale calculations, if the results are up-scaled. Secondly, the fields originating from the two different models might be fed into the same diagnostic tool, e.g. the on-line calculation of the radiative forcing calculated consistently with the same radiation scheme. Last but not least, enabling the 2-way data transfer between two models is the first important step on the way to a fully dynamically and chemically 2-way coupling of the various model instances.

In MMD (v1.0) interpolation between the basemodel grids is performed via the COSMO pre-processing tool INT2LM, which was implemented as MMD submodel for on-line interpolation, specificially for mapping onto the rotated COSMO grid. A more flexible algorithm is required for the backward mapping. Thus, MMD (v2.0) uses the new MESSy submodel GRID for the generalised definition of arbitrary grids and for the transformation of data between them.

In this article we explain the basics of the MMD expansion and the newly developed generic MESSy submodel GRID (v1.0) and show some examples of the applications mentioned above.

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1 Introduction

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As fifth part of a paper series about the MECO(n) system and as such as a component of the ACP / GMD special issue¹ about the Modular Earth Submodel System (MESSy), this article documents a progress of the MESSy code development. More specifically, the second generation of the Multi-Model-Driver (MMD v2.0) is introduced enabling the 2-way on-line nesting between different model instances (basemodels). Thus On-line nesting means that the coupled models exchange their data via the computer memory, in contrast to the data exchange via files on disk in common off-line nesting procedures. Thus, this article describes a further development of the 1-way on-line nesting system presented in the second part of the paper series (Kerkweg and Jöckel, 2012b).

We achieve the nesting by coupling different models, thus our 2-way nesting is implemented as 2-way coupling of global and regional atmospheric models. Usually the term "2-way coupling" is used in the context of different Earth system compartment models, such as land, ocean or atmospheric models being connected within a comprehensive Earth System Model. Here, 2-way nesting through 2-way coupling is used to distinguish it from fundamentally different other nesting techniques, as for instance local static grid refinement. For a number of atmospheric models grid refinement features exist. Usually, the grid resolution needs to be subdivided by a fixed factor: e.g., 3 for the WRF model (Moeng et al., 2007; Harris and Durran, 2010) or 2 for the ICON model (Zaengl et al., 2015). These constraints minimise the interpolation error, at least for the horizontal interpolation. Additionally, these models, at least the two mentioned above, deal with the grid refinement areas as different, so-called "patches" within the same executable, i.e., they are coupled "internally" (see Kerkweg and Jöckel (2012b) for a discussion of internal and external coupling). In contrast to this, the MECO(n) (MESSy-fied ECHAM and COSMO models nested n-times) system is implemented as an external coupling, i.e., a real 2-way nesting of the same or different basemodels (here COSMO/MESSy and EMAC).

In the MECO(n) system we follow this second approach for the following reasons:

- Different It is necessary to couple the model instances externally, as different basemodels, EMAC and COSMO/MESSy, are nested into each other, which. This in itself prevents the "patches approach", i.e., it is necessary to couple the model instances externally. as the internal coupling or "patches approach" is usually a feature of regional grid-refinements, which is directly embedded in (or part of) the model code, as for instance in WRF or ICON, in which the user can specify the number of patches and their corresponding domains flexibly at run-time. For such a feature, however, the entire model code needs to be "aware" of a(n arbitrary) number of grid-refined patches. To equip legacy code (as COSMO or ECHAM) supplementarily with such a feature would basically mean to rewrite the entire code from scratch. The reason is that all prognostic (and diagnostic) variables need to exist on each patch technically independent of each other.
- Different COSMO/MESSy model instances are nested into each other using the same algorithms as for the EMAC-COSMO/MESSy nesting. The external coupling approach was favoured here, due to limitations of the Fortran95 name-space: In fully object oriented languages, overloaded "sets" or "instances" of the same variable(s) could be defined, however, the Fortran95 language standard does not allow to have the same variable with the same name in the

¹http://www.geosci-model-dev.net/special_issue10_22.html

same name-space more than once. Thus a complete recoding of the basemodel, e.g., replacing arrays by structures of arrays, would be required for the patches approach.

- A nesting of COSMO/MESSy model instances employing different grids (e.g., rotated differently) is possible. This also includes the possibility to realise an arbitrary resolution jump, i.e., the factor for the grid refinement is freely selectable, in contrast to the fixed factors of 2 or 3 as required by the ICON or the WRF model, respectively. Especially, for air quality applications a higher resolution jump is necessary to reduce computational costs. Here, a global instance providing consistent boundary data is required, while the scientific focus is on a much finer resolved model instance.
- Due to the external coupling, prognostic variables are not necessarily all coupled back to the coarser model. Thus, 2-way nesting does not necessarily imply (full) feedback of the smaller to the coarse scale model. Consequently, the coupling can also be used to couple back diagnostic fields only. Additionally, testing of the influence of the coupling of different (individual) variables is easier to accomplish by external coupling.

Apart from these advantages, the external coupling proves to be more challenging than the internal coupling. Horizontal and vertical interpolation errors are expected to be larger, depending on the relations between the different grids and differences in their orographies. From these, the adaption to the higher resolved orography of the nested simulation, causes the largest error. An additional disadvantage of all external coupling approaches is the need for the user to optimize the distribution of the available parallel tasks among the different model instances, in order to achieve an optimum run-time performance with minimized waiting times between the model instances.

As far as we know, the only other 2-way on-line nested modelling system using external coupling is an MPI-ESM ² (Giorgetta et al., 2013) - COSMO-CLM coupling via OASIS3-MCT (Weiher et al., 2016) (Will et al., 2017). This was developed in parallel to our 2-way coupling approach within the same BMBF funded MiKlip project², as different approaches had to be assessed. In contrast to our system, the MPI-ESM - COSMO coupling via OASIS3-MCT is restricted to the coupling of one COSMO instance only, i.e., no further on-line COSMO - COSMO coupling is possible in the system of Weiher et al. (2016) Will et al. (2017). Technically, this COSMO - COSMO coupling would of course also be possible, but it is not implemented. In the rest of the article, we will use the terms "2-way coupling" and "2-way nesting" synonymously for the approach chosen in the MECO(n) system.

This article documents a major achievement in the development of the on-line coupled MECO(n) system, which central part is the MESSy software: As described by (Jöckel et al., 2015; Baumgaertner et al., 2016, and the MESSy homepage: http://messy-interface "The Modular Earth Submodel System (MESSy) is a software providing a framework for a standardized, bottom-up implementation of Earth System Models (or parts of those) with flexible complexity. "Bottom-up" means, the MESSy software provides an infrastructure with generalized interfaces for the standardized control and interconnection (=coupling) of "low-level ESM"

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²"A special issue of the Journal of Advances in Modeling Earth Systems (JAMES) will be dedicated to the initial description of the MPI-ESM, through numerous papers (currently in review) by MPI-M researchers." Cited from the web site of the Max Planck Institute for Meteorology, Germany, hosting the model (last access date: 29.09.2016)

²https://www.fona-miklip.de/

components" (dynamic cores, physical parameterizations, chemistry packages, diagnostics etc.), which are called submodels. MESSy comprises currently about 60 submodels (i.e., coded MESSy conform):

- infrastructure (= the framework) submodels (sometimes called generic submodels),
- diagnostic, atmospheric chemistry and model physics related submodels.
- The main design concept of MESSy is the strict separation of process description (=process and diagnostic submodels) from model infrastructure (e.g., memory management, input/output, flow control, ...).

Within MESSy, the operator splitting is formalized as the fundamental concept. Model codes are organized in 4 conceptual software layers: a basemodel of any level of complexity is complemented by a basemodel interface layer (BMIL). A further interface layer to the submodels (SMIL, submodel interface layer) makes it possible to keep process submodels as distinct as possible in the submodel core layer (SMCL). (Cited from Jöckel et al., 2015; Baumgaertner et al., 2016, and the MESSy homepage: http://messy-in MESSy currently employs the programming language Fortran90/95 with some rare exceptions linking libraries containing C or C++ code.

Furthermore, different basemodels, e.g. the global model ECHAM³, the regional COSMO model⁴, and the coupled global climate model CESM1⁵ have been expanded by the MESSy middleware (i.e., the MESSy infrastructure components) to enable a standardised expansion by additional or alternative process components (e.g. for physics or chemistry) and diagnostic components, which we call MESSy submodels.

In Part 2 of the MECO(n) model documentation the 1-way on-line coupled model system MECO(n) (MESSyfied ECHAM and COSMO models nested n-times) for which MMD was developed initially, was described in detail (Kerkweg and Jöckel, 2012b). In the on-line coupled system MECO(n) an arbitrary number of COSMO/MESSy model instances are nested on-line into one master model. This driving model can be either the global EMAC or a coarser COSMO/MESSy model instance. On-line nesting means that the coupled models exchange their data via the computer memory, in contrast to the data exchange via files on disk in common off-line nesting procedures. The data exchange is implemented as client-server system, where the driving model acts as server providing the client model with the data required for the calculation of the inital and boundary fields used to drive the regional model.

³The core atmospheric model is the 5th generation European Centre Hamburg general circulation model (ECHAM5, Roeckner et al., 2006). The ECHAM/MESSy Atmospheric Chemistry (EMAC) model is a numerical chemistry and climate simulation system that includes sub-models describing tropospheric and middle atmosphere processes and their interaction with oceans, land and human influences (Jöckel et al., 2010).

⁴COSMO is the regional weather prediction model of the Consortium for Small Scale Modelling (COSMO model, Steppeler et al., 2003; Doms and Schättler, 1999) and the community model of the German regional climate research (Rockel et al., 2008). By implementing the MESSy interface the COSMO model was expanded to a regional chemistry (climate) model (Kerkweg and Jöckel, 2012a; Mertens et al., 2016).

⁵The Community Earth System Model version 1.2.1 (CESM1) is a fully coupled climate model. *CESM is sponsored by the National Science Foundation* (NSF) and the U.S. Department of Energy (DOE). Administration of the CESM is maintained by the Climate and Global Dynamics Laboratory (CGD) at the National Center for Atmospheric Research (NCAR) (cited from http://www.cesm.ucar.edu/models/cesm1.0/., last access date: 27.09.2016) (Hurrell et al., 2013; Baumgaertner et al., 2016)

The Multi-Model-Driver (MMD v1.0) provides the software necessary for the data exchange from the server to the client model and for the calculation of the initial and boundary data. MMD consists of two parts: (1) a library which performs the data exchange between the model instances, and (2) MESSy submodels, which organise and process these data.

In addition to the functionalities provided by MMD (v1.0), the update of MMD presented here, provides the possibility to exchange data in both directions during the time integration phase of a simulation. For the unidirectional data exchange the expanded INT2LM⁶ software was used to interpolate the data from the driving model grid to the target model grid. This software is a specialised software for the calculation of the initial and boundary data of the COSMO model. Therefore, a different software is required to interpolate the data from the finer to the coarser grid for the data sent from the client model to the server model. According to the MESSy philosophy of strict separation and generalisation, we therefore developed the new generic submodel GRID (v1.0), which is also documented in the present article. GRID is can be used for all grid mapping operations required during a simulation.

In the next section we describe the new developments within MMD. As the data mapping between the different grids is central to this further development of MMD, Sect. 3 introduces the newly developed GRID submodel, which provides the required mapping functionalities —used for the remapping from the finer to the coarser model instance. Some examples for 2-way data exchange are shown in Sect. 4. A brief run-time performance analysis of the model is presented in Sect. 5.

2 The Multi-Model-Driver (MMD v2.0)

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The Multi-Model-Driver is the coupling software performing the data transfer between two independent basemodels running within the same MPI environment. Appendix A of Kerkweg and Jöckel (2012b) provides an overview about different coupling approaches, especially the differences between *internal* and *external coupling* are discussed. Furthermore, Sect. 4 of Kerkweg and Jöckel (2012b) explains why MMD was chosen as coupling software between different MESSy basemodels. In summary, apart from the reasons named already in the introduction, MMD provides the best balance between fast data transfer and the possibility to integrate model specific software, such as INT2LM into the coupling procedure. INT2LM is the software provided by the German Weather Service (Deutscher Wetterdienst, DWD) for the calculation of the initial and boundary data for the regional COSMO model. This software was included into MMD (v1.0) as subsubmodel INT2COSMO.

INT2LM and thus INT2COSMO does not only include the interpolation routines to map the driving model fields to the regional model grid. It furthermore processes the external data required as input to the COSMO model and provides the calculation of additional fields required by the COSMO model, which are not necessarily provided directly by the driving model.

The coupling was implemented following a client-server approach. Therefore, in MMD (v1.0) all routines and modules have been named server (serv) or client (clnt) in accordance to the model using them. In MMD (v2.0) the routines and modules have been renamed to parent and child instead of server and client. This is reasonable was required, as the term server implies that

⁶see Part V of the COSMO model documentation http://www2.cosmo-model.org/content/model/documentation/core/default.htm, last access date: 29.09.2016

this model is sending the data. As in MMD (v2.0) data are sent in both directions, the terms parent and child for the coarser and the finer model, respectively, are better suited.

30 MMD consists of two parts:

- 1. a library performing the data tranfer, which is independent from the coupled models, and
- 2. the part for data provision and processing implemented as MESSy submodels.

The library was extended by a few subroutines enabling the data transfer in both directions. The larger changes occured in the MESSy submodels, as the data processing routines for the back transfer of the data had to be implemented. In the following subsections an overview about the changes and additions made within these two parts of MMD are described. The MMD library Manual and the MMD User Manual in the Supplement provide all technical details about the implementation.

2.1 The MMD (v2.0) Library⁷

The Multi-Model-Driver (MMD) library manages the 2-way data exchange between the different tasks of one EMAC and/or an arbitrary number of COSMO/MESSy instances as illustrated in Fig. 1. The configuration of the client-server system is defined in the Fortran95 namelist file MMD layout.nml (which is written automatically by the run-script). This namelist file contains the information about the overall number of model instances within the current MECO(n) setup (i.e., n+1), the number of MPI tasks assigned to each model, and the definition of the parent model of the respective model (for further details see the "MMD (v2.0) library manual" in the Supplement). The library contains a high-level API for the data exchange between the different models. Figure 2 illustrates the functional principle of the MMD library. During the initialisation phase, the exchange of information required by the parent from the child model and vice versa, is accomplished by utilising the MPI routines MPI send and MPI recv. During the integration phase, data can be exchanged in both directions, i.e. from the parent to the child model and vice versa. Point-to-point, single-sided, non-blocking communication is applied to exchange the required data between the different MPI-tasks. For longer simulations, check-pointing is required "Check-pointing" (the technical term for "restarting") is required (not only for climate simulations) to be able to continue a simulation after hardware failures, for branching off sensitivity studies, and last but not least, it is required to split a simulation into parts, fitting into the typical time limits of a job scheduler on a super-computer. To enable check-pointing, one additional communication step occurs during the integration phase: for the synchronisation of the models w.r.t. the check-pointing, the parent model has to send the information whether the simulation will be interrupted after the current time step. This data exchange is implemented as direct MPI communication using MPI_send and MPI_recv. As the routine MPI_alloc_mem, used to allocate the memory (buffer) required for the data exchange, can only be used in C (and not in Fortran95), some parts of the MMD library are written in C, however most parts are written in Fortran95 for consistency with the POINTER arithmetic used for the MESSy memory management (see Jöckel et al., 2010). The MMD library routines and their usage are described in detail in the "MMD (v2.0) library manual" (see Supplement).

⁷The text of this section is adopted from the initial publication of the MMD library in Kerkweg and Jöckel (2012b).

2.2 The MESSy submodel MMD2WAY

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In addition to the library, the MMD software comprises a regular MESSy submodel as "wrapper". This submodel provides and processes the data transfered by the library. MMD (v1.0) contained two MESSy submodels: one for the server (MMDSERV) and one for the client (MMDCLNT). Here, the server controls the timing of the client model and "serves" the data, which is processed by the client. In the new MMD version, the client also provides data to the server model. As the difference between the models with respect to the data transfer is thus only the time control of the models, the server and client models have been renamed to parent and child models, thus omitting the impression that only the server acts as "data server". Thus the new MESSy submodel MMD2WAY has been implemented. It consists of two submodels: MMD2WAY_PARENT and MMD2WAY_CHILD. These sub-submodels subsubmodels provide the same functionalities for the 1-way on-line coupling as MMDSERV and MMDCLNT in MMD (v1.0), respectively. This is described in detail in Part 2 of the MECO(n) model documentation (Kerkweg and Jöckel, 2012b): In the initial phase of a model simulation

- the parent imprints its time settings on the child model; these are end-date, restart trigger, and, at the very first start of a
 model instance, the (re-)start-date as start-date of this instance.
- the fields required from the parent are read from the &CPL_CHILD_ECHAM or &CPL_CHILD_COSMO namelist in the mmd2way.nml namelist file for ECHAM or COSMO as parent models, respectively. The names of the parent fields are sent to the parent, and in both models pointers to the respective data fields and dimension informations are set.
- the exchange matrix, the so-called "index list", is set up. This index list provides the information, which grid box (index pair (i_p, j_p) on which parent parallel task (PE_p) exchanges data with which child grid box (i_c, j_c) on which child parallel tasks (PE_c). For this, the child model has to define an "in-grid". This is a sub-area of the parent grid (i.e., it has the same rotation and the same mesh size) and completely overlays the child grid. Fig. 3 illustrates the relation between the different grids. Afterwards the data is transformed from the in-grid to the child grid using INT2COSMO⁸ the expanded version of the preprocessing software INT2LM for the COSMO model (INT2COSMO, see Kerkweg and Jöckel, 2012b, for further explanation

During the integration phase, the MMD library sends the data from the parent model to the child model. The child model calculates the required initial and boundary conditions from the parent data and transforms additional data to the child grid.

This functionality for the 1-way coupling is kept the same in MMD (v2.0). In addition, MMD2WAY_PARENT and MMD2WAY_CHILD have been expanded for the data transfer from the child to the parent model. For most functionalities of the 1-way coupling a counterpart for the data transfer in the other direction could be implemented by keeping the same logic. Thus, a namelist (&CPL_PAR_CHILD) in the parent model namelist file mmd2way.nml determines, which fields are exchanged between the child and the parent model. In the initial phase of a model simulation this information is transferred to the child model. Both models set pointers to their corresponding data objects. Again, the child model has to define a grid, which is a subpart of the parent model grid (called "out-grid"), and it has to perform the data transformation from the child model grid

⁸INT2COSMO is the expanded version of the preprocessing software INT2LM for the COSMO model.

to the out-grid. The decision to transform the data within the child model was taken in order to minimize the amount of data to be transferred between the models: as the parent model grid will usually be coarser resolved, data on this grid is exchanged via MMD. For the transformation from the child to the out-grid, the newly written MESSy infrastructure submodel GRID is used (see Sect. 3). At the First, the data is remapped horizontally, before the vertically remapping procedes in an extra step. For the time being, only conservative remapping is implemented as transformation method. , as provided by GRID, is utilized as horizontal transformation method in MMD2WAY_CHILD. As the COSMO model uses a staggered Arakawa-C grid, the wind components need to be interpolated to the grid midpoints prior to the horizontal remapping for the COSMO-EMAC coupling, as the EMAC wind components are defined on the grid midpoints. For the COSMO-COSMO coupling the wind components are interpolated directly between the staggered grids, i.e., they are always defined on the box edges.

The vertical remapping differs dependent on the parent model. If EMAC is the parent model, NREGRID is used for the vertical remapping of the fields. In this case, data of a non-hydrostatic model with a fixed vertical geometry need to be converted for a hydrostatic model using hybrid pressure coordinates. The vertical coordinate in the COSMO model is defined as a pseudo-hybrid pressure axis. For this the hybrid coefficient calculation as provided by INT2LM is used as input vertical axis to the vertical interpolation via NREGRID. Furthermore, the new surface pressure in the EMAC model is approximated by an iterative calculation of the pressure, temperature and humidity (vapour, liquid water and cloud ice) vertical profiles. For the vertical interpolation of the COSMO-COSMO coupling, the INT2COSMO spline-interpolation is used.

The intepolated data is sent to the parent model, where it is subsequently weighted (if requested) and assigned to the target parent model fields.

For the utilisation of the child data by the parent model, two methods are distinguished:

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"0": for purely diagnostic applications: the field is only used as input to the parent model, i.e., this field is created by the coupling submodel and thus independent of other model data objects. In this case, the memory is allocated by MMD2WAY PARENT, and the transferred field is copied to this memory without any further modifications.

1: the

- 20 "1": for feedback from the finer to the coarser resolved model instance: the exchanged field is used to modify an existing directly modify a parent model field. Therefore, no additional memory needs to be allocated by MMD2WAY_PARENT.

 Using method 1, there are two options for modifying a prognostic variable of the parent model:
 - (a) the value of the variable can be changed directly, or
 - (b) the tendency of the variable can be modified.
- 25 For all non-prognostic variables only option (a) is possible.

For both options, a weighting between the original value of the parent field (P) and the child model field (C) is applied:

$$P(i,j,k,tlev) = P(i,j,k,tlev) * (1. - f_{mn} * f_{vw}(k) * f_w(i,j)) + C(i,j,k,1) * f_{mn} * f_{vw}(k) * f_w(i,j)$$
(1)

Here, i and j are the indices along the horizontal dimensions, k the index along the vertical dimension, and tlev indicates (if applicable) the respective time level.

The different weight coefficients are:

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- f_{mn} is the relaxation strength. Its value is set in the parent namelist individually for each field.
- f_{vw} is a vertical weight function. It depends on the vertical index k. In most cases the domain coupled back from the child model does not cover the full height of the parent model⁸. To avoid artificial jumps in the data fields, a weight function is required, which gradually decreases from 1 in the core domain to zero towards the edge of the domain. The weight function is implemented as a cosine function:

$$f_{vw}(k) = 0. for \ k <= k_{min}$$

$$f_{vw}(k) = cos\left(\frac{\pi}{2} * \left(1 - \frac{k - k_{min} - 1}{n_k - 1}\right)\right)^2 for \ k_{min} < k <= k_{min} + n_k$$

$$f_{vw}(k) = 1. for \ k > k_{min} + n_k$$
(2)

In Eq. 2 it is assumed that the vertikal index k increases from top to bottom; k_{min} is the height index of the top of the child domain, n_k is the number of vertical layers the cosine function should cover.

- f_w is the horizontal weight function: This weight function is required to avoid artificial jumps at the borders of the area, where the fields are relaxed to the child variables. Currently, the user can choose between three different implementations by namelist:
 - 0: f_w is set to 1 everywhere in the child domain. This option is for testing only, as it may lead to artificial jumps in the data.
 - 1: f_w is implemented as the sum of two cosine functions:

$$f_w(i,j) = 1. - (\cos(x)^e + \cos(y)^e)$$
 with $x = \pi * \frac{i}{i_{max}} ; y = \pi * \frac{j}{j_{max}}$ (3)

 i_{max} and j_{max} are the number of grid points in the two horizontal directions, respectively. The exponent e is set by namelist. Its default value is 14.

2: f_w decreases in the form of a cosine from 1 in the domain inner part to 0 at the borders of the coupled domain. The width of the damping zone is determined by a namelist parameter damprel. Its valid range is [0, 0.5].

⁸e.g., in the case of the COSMO/MESSy model, only the data below the damping layer should be coupled back.

This number determines the relative width of the damping zone. If, for example, damprel = 0.2 for a model domain consisting of 100 grid boxes in x-direction (index i) and of 50 grid boxes in y-direction (index j), the damping zone in x-direction is 20 grid boxes wide, and in y direction 10 grid boxes wide, respectively.

All these weight functions are defined on the child grid. They are once, during the intialisation phase, transformed in the same way as the data are transformed, and sent to the parent model for application during the integration phase. Figure 4 displays the different weight functions for a domain over Europe. The upper row shows the weight functions as defined on the child model grid. Note, that the coupled domain is smaller than the child domain (with the exception of $f_w = 0$). This is because the damping zone of the regional model itself should not be coupled back to the parent model, as this is, for 2-way coupled variables, directly influenced by the parent model and thus spurious damping or amplifications could occur. The lower row of Fig. 4 shows the same weight functions after the transformation to the parent grid.

If the tendency is subject to change (i.e., method 1, option (b) is used), first the current value of the parent field (*P*) needs to be calculated from the values at the previous time step plus the tendencies of the current time step. This field is modified according to Eq. 1 and an additional tendency is calculated from the difference between the parent fields before and after the modification.

3 The generic MESSy submodel GRID (v1.0)

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- The generic MESSy submodel GRID provides the basis for all required grid transformations during a MESSy simulation. Ideally Due to the increasing complexity of Earth System Models, grid transformations at run-time of the model, (e.g., remapping from an atmosphere grid to a higher resolved land grid and vice versa) are more and more commonly required. To avoid serveral implementations throughout the code, such an on-line transformation functionality is implemented as a central (remapping) functionality should be implemented as one important part of the models model infrastructure, providing a common grid processing functionality. This includes the routines for grid definition, grid modification, and the transformation between different grids. Implementation of this functionality as one central important part of the model infrastructure simplifies the maintenance and expansion of the functionality, because it is utilised jointly by all model components. As the infrastructure module is written in a general way, performance optimisation or additional grid types, transformation algorithms, etc. can be implemented straightforwardly. Ideally the final version provides should provide
- the treatment of different grid-types:
 - Spatial grids are usually 2-D or 3-D in space. Different types of horizontal grids can be distinguished, such as:
 - regular rectangular grids, which are either orthogonal in geo-coordinates or rotated grids, and (rectilinear grids) or curvi-linear grids.
 - irregular grids⁹non-rectangular structured grids⁹, and

⁹The implementation of irregular grids is ongoing and thus not yet part of GRID v1.0.

⁹The implementation of non-rectangular, structured grids is ongoing and thus not yet part of GRID v1.0.

• unstructured grids.

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The 3-D spatial grids consist of one of the above mentioned horizontal grids and of a vertical dimension. The vertical axis can be defined in different ways, e.g., as height or pressure based coordinate.

- Additionally the time might also be considered as part of the grid, thus treatment of 4-D grids (i.e., 3-D in space + a time axis) might be considered.
- depending on the application, different grid-transformations for different grid-types, such as
 - conservative remapping, and
 - (not necessarily conservative) interpolation.
- 5 Moreover, the code of the desired infrastructure module following this design concept must be
 - well structured to support flexible expansions,
 - as simple as possible, to keep it maintainable,
 - efficient, i.e., show a good run-time performance and therefore, it must work in a parallel environment and scale appropriately, and
- designed to cause an as small as possible memory foot print during operation.

The infrastructure submodel GRID¹⁰ constitutes such an infrastructure model for MESSy providing the grid definition sturctures structures and transformation routines.

For a grid transformation, first the source and the target grid need to be defined. Second, the transformation remapping of data between these grids can be calculated. These Not all of the above listed functionalities are implemented in GRID yet. The following two subsections provide an overview of the functionalities provided currently by GRID. Their implementation in GRID is organised as follows:

- The SubModel Core Layer (SMCL) of GRID provides a unified interface for the definition of all grids required in all MESSy submodels. It is implemented as a Fortran95 structure, which contains all required information of a grid in a generalised way.
- The subsubmodel GRID_TRAFO provides the interface routines to use these grid information for the transformation between the different grids. GRID_TRAFO utilises third party grid transformation codes: currently NREGRID¹¹ (Jöckel, 2006) and SCRIP (Jones, 1999).

The next two parapraphs provide a short overview of the content of the generic MESSy submodel GRID. The "GRID User Manual" in the Supplement provides detailed information about the usage of the GRID submodel.

¹⁰The names of MESSy submodels are written in capital letters throughout the articleeven, even though they are not necessarily acronyms.

¹¹ Note: The infrastructure submodel previously used in EMAC is named NCREGRID, while the remapping algorithm itself is called NREGRID.

25 3.1 The SubModel Core Layer of GRID

ESMs Earth System Models usually infer grids in spherical geometry. Three different grid types are distinguishable: (1) regular rectangular grids, which are orthogonal in geo-coordinates, (2) regular orthogonal rotated grids(i.e., curvi-linear in geo-coordinates) curvi-linear grids, and (33) non-rectangular, structured grids, and (4) unstructured or irregularly geo-located grids.

Most of the internal data types of GRID follow the netCDF data model. The hierarchical data structures follow mainly those of NCREGRID (Jöckel, 2006). The definition of the so-called "Fortran structure, which contains all components required for the definition of a geo-hybrid grid" structure, was extended and generalised for the usage in GRID. During a model simulation, the definition of an arbitrary number of geo-referencing grids and the transformations between those grids are possible. A gridis horizontally defined by geographical longitude and latitude and vertically by hybrid pressure coefficients The geo-hybrid grid, as defined by Jöckel (2006), consists of a horizontal grid space, which comprises geographical latitude and longitude of the mesh vertices and / or centers. For different types of grids, different structures structure components for the definition of the horizontal grid are specified. The GRID vertical grid space is defined in analogy to the hybrid pressure level definition. Depending on the setting of the coefficients and of the reference and surface pressure, the vertical axis can be defined as one of (1) pressure hybrid pressure axes, (2) constant pressure axes, (3) constant height axes, or (4) sigma levels. More details can be found in the GRID User Manual in the supplement.

The GRID SMCL routines also comprise subroutines for the handling of the grid structures, i.e., routines for initialising, copying, importing, exporting and printing a variable of the grid structure type. Beyond that, routines necessary for defining a grid, storing it in a concatenated list, locating an already defined grid within this list, and for comparing grids, are part of the GRID SMCL. During a model simulation, the definition of an arbitrary number of geo-referencing grids and the transformations between those grids are possible.

3.1.1 GRID TRAFO

The main intention of the GRID_TRAFO submodel is to provide routines for the transformation of gridded geo-located data. GRID_TRAFO comprises the in EMAC well established standard remapping tool NREGRID (Jöckel, 2006) and the SCRIP¹² software (Jones, 1999). While NREGRID is restricted to mapping between orthogonal 2-D or 3-D grids, SCRIP provides transformations to / from curvi-linear or unstructured grids. Here, we use grid "transformation" as generic term for both, conservative remapping (or "regridding") as well as for (not necessarily conservative) interpolation.

The "geo-hybrid grid "-structure provides all information required for the grid conversion. As each remapping software (NREGRID and SCRIP) relies on its specific structure grid information, GRID_TRAFO additionally provides routines to extract this as required by the respective mapping software, i.e., it provides the "middleware" or acts as "wrapper" for the established mapping software. The remapping algorithms automatically apply the correct conversion routines, depending on

¹² Spherical Coordinate Remapping and Interpolation Package

the associated structure components. While the core mapping algorithms differ, GRID_TRAFO provides unified interfaces for the conversion between different grids. Additional interpolation schemes can be easily added, if required in the future.

The details are explained in the "GRID User Manual", which is part of the Supplement.

30 **3.1.2 NREGRID**

The remapping algorithm NREGRID is a recursive algorithm, which is applicable to arbitrary orthogonal (including curvilinear) grids of any dimension. The algorithm does not apply a point-to-point interpolation, but a transformation based on overlapping volumes between the different grids. It is for the rediscretisation of "gridded" geo-scientific data between n-dimensional (usually n = 2 or 3) orthogonal grids. The conservative rediscretisation of extensive or intensive variables is based on the calculation of the overlap (area or volume) matrix between source and destination grid boxes. For orthogonal grids these overlap matrices can nicely be calculated recursively, since the overlap area / volume is zero as soon as at least the overlap interval along one axis (dimension) is zero. Since the recursive nature of this algorithm limits its application to orthogonal grids, it cannot be applied for rediscretisations between the (in geographical coordinates) orthogonal Gaussian grid of ECHAM5 and the rotated (in geographical coordinates non-orthogonal) COSMO grid.

Details about the NREGRID algorithm have been published by Jöckel (2006).

3.1.3 SCRIP

As NREGRID is limited to the remapping between equally oriented orthogonal grids, the implementation of an algorithm able to transform between different curvi-linear or even unstructured grids became necessary. For this, the SCRIP software 13 (Jones, 1999) version 1.4 provided by the Los Alamos National Laboratory has been utilised. SCRIP (a Spherical Coordinate Remapping and Interpolation Package) "is a software package used to generate interpolation weights for remapping fields from one grid to another in spherical geometry. The package currently supports four types of remappings. The first is a conservative remapping scheme that is ideally suited to a coupled model context where the area-integrated field (e.g. water or heat flux) must be conserved. The second type of mapping is a basic bilinear interpolation which has been slightly generalized to perform a local bilinear interpolation. A third method is a bicubic interpolation similar to the bilinear method. The last type of remapping is a distance-weighted average of nearest-neighbor points. The bilinear and bicubic schemes can only be used with logically-rectangular grids; the other two methods can be used for any grid in spherical coordinates." (Quoted from: SCRIP Users Guide, Introduction, Jones, 1998).

3.1.4 Application of GRID in MMD2WAY_CHILD

The COSMO model uses a rotated grid and the orientation between two COSMO model instances or the COSMO and the EMAC model is arbitrary. As NREGRID requires equally oriented orthogonal grids, it is not applicable in MMD2WAY. Sadly,

¹³http://oceans11.lanl.gov/trac/SCRIP (last access: 23 June 2015 18 October 2017). The official link named in the SCRIP users guide (http://climate.acl.lanl.gov/software/SCRIP) is not available anymore.

SCRIP provides only algorithms for horizontal grid transformation. Thus two steps are required for the remapping of 3D-3-D data fields. First

Usually the biggest problem in 2-way nesting of two atmospheric models, is the height correction required due to the differently resolved orographies of the child and the parent model. Thus, it seems to be a natural choice to first regrid horizontally and to perform the vertical regridding intertwined with the height adjustment as a second step. Therefore, first, horizontal remapping via SCRIP was conducted, secondly, is conducted. In a second step, the vertical remapping is performed using NREGRID for COSMO-EMAC coupling. For the COSMO-COSMO coupling, it was decided to use the INT2COSMO spline-interpolation. Nevertheless, additional vertical interpolation schemes can be easily added if required in the future.

5 3.2 The BaseModel Interface Layer of GRID

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The backbone of each model is its grid, e.g., for an atmospheric model, the horizontal domain is given by a definition of the geographical longitudes and latitudes of the models grid midpoints and the grid corners. The vertical dimension is usually defined by a height or pressure based coordinate. As this grid (called "basegrid" in the following) is the reference for most submodels and processes, the basegrid is defined in the basemodel interface layer (BMIL) for the usage in all MESSy submodels. In case of MMD2WAY, MMD2WAY CHILD utilises the basegrid as source grid for the mapping to the "out-grid".

4 Example Applications using the 2-way coupled MECO(n) system

As discussed above, two different types of vertical interpolation routines are used for the two directions in MMD (v2.0): for the parent-to-child data transfer the spline interpolation of <a href="https://linear.com/interpolation-interpolat

Nevertheless, the current implementation allows for some handy useful applications, e.g., data can be transferred on-line from the finer to the coarser grid to compare data on the coarse grid. A simple example is provided in Sect. 4.1. Additionally, diagnostic tools —can be used to interpret global and regional model results consistently, e.g. for radiative forcing, which is consistently determined only, if calculated with the same radiation code. Section 4.2 illustrates this utilising the radiative forcing calculations of EMAC.

As discussed in Sect. 2.2, the 2-way coupling of prognostic variables is technically implemented in the MMD2WAY sub-model. Thus Sect. 4.3.1 provides an example for an EMAC - COSMO/MESSy coupling, where dust tracers are coupled 2-way. Finally, Sect. 4.3.2 shows the full dynamically 2-way coupling of two COSMO/MESSy model instances located over the Atlantic ocean (i.e., over flat terrain) using the same height coordinates. The results indicate that the 2-way coupling has the potential to improve the representation of hurricanes in the coarser COSMO/MESSy model instance.

4.1 Simple examples of added value through aggregated subgrid-scale information

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Depending on their resolution, atmospheric models can resolve only certain processes, whereas others have to be parameterised. Naturally, smaller scale models can resolve more processes explicitly. For 2-way applications the questions The question, if the aggregation of the subgrid-scale information provided by the smaller scale model to the larger scale model constitutes an added value for the larger scale model is still under debate and might be answered with the help of 2-way coupled applications. Most probably, the answer will differ for different processes. For some dynamical processes, e.g. the generation of Rossby waves or Hurricanes (see Sect. 4.3.2), the upscaling might result in an added value, as these phenomena originate from smaller scale disturbances.

For chemical models, especially the treatment of emissions is of interest. On the one hand, emissions, which depend on soil properties and/or on prognostic variables in the model (the so-called on-line emissions, because they are calculated during the simulation), can substantially differ between models with different resolution. One example are dust emissions, which depend on the 10m wind speed, soil properties and soil moisture (see Sect. 4.3.1). On the other hand, it is normally assumed, that even point and line emissions are instantly mixed within the grid box into which they are emitted. This leads to a higher dilution in larger scale models. Especially in highly polluted regions, or more generally near emission sources, this might influence the simulated chemical regime, as atmospheric chemistry is highly non-linear.

Figure 5 illustrates, as a simple example, the effect on on-line calculated NO nitrogen oxide (NO) soil emissions (Kerkweg et al., 2006b). These emissions strongly depend on the soil properties and thus differ substantially between the models.

Panel A depicts the NO emission flux as calculated on a global EMAC model grid of T42 ($\approx 2.8^{\circ}$) resolution. Panel B shows how these emission fluxes look on a COSMO/MESSy grid with 0.36° horizontal resolution. If COSMO/MESSy is were 2-way coupled into EMAC and EMAC would use were using the NO emissions coupled from COSMO/MESSy instead of calculating them itself, the emissions aggregated from the COSMO/MESSy to the EMAC grid would be as in Panel C. Panel D depicts the difference in percent between the emissions directly calculated by EMAC (Panel A) and coupled back from COSMO/MESSy (Panel C). Naturally, the emission fluxes on the COSMO/MESSy grid show much finer structures as a result of the finer grid and thus finer distributed soil properties. However, the largest differences between the up-scaled (Panel C) and in EMAC calculated (Panel A) emission fluxes occur at the coast lines (Panel D), what which is mostly due to the much finer resolved land-sea mask in the smaller-scale model. The NO emission flux integrated over the coupled domain is 3.29kg(NO)/s and 2.63kg(NO)/s for the parent and the child model, respectively. Thus, the differences in the soil properties of the two models account for a difference of 0.66kg(NO)/s. The integrated NO emission flux regridded from the child to the parent grid is 2.78kg(NO)/s, providing an emission flux lower by 0.51kg/s compared to the directly calculated integrated emission flux. The difference of 0.15kg(NO)/s between the flux on the regional domain and its integral on the global domain, respectively.

As a second example, the dry deposition velocities for ozone are displayed in Fig. 6 (Kerkweg et al., 2006a). The features discussed for the pervious example appear here as well. Additionally, the ozone dry deposition velocities calculated by COSMO/MESSy are much more evenly distributed in the Mediterranean region, while they are slightly but systematically

smaller over Eastern Europe, which is most propably due to different soil properties in that region and also due to the different turbulence schemes employed by the two basemodels.

4.2 Use of specific diagnostic tools: radiative forcing

To evaluate the radiative forcing for two MECO(n) instances consistently, the MESSy submodel RAD (Dietmüller et al., 2016) is used for the calculation of the radiative forcing of a nested COSMO/MESSy instance within on-line coupled to the EMAC model. As COSMO/MESSy and EMAC use different radiation schemes, this is one way of a consistent comparison.

Here, results are shown from simulations using a setup as published by Mertens et al. (2016). A COSMO/MESSy instance over Europe (0.44° resolution) was nested in coupled to the global EMAC domain. The ozone field calculated by COSMO/MESSy was sent back to EMAC using MMD. However, the ozone field coupled back from COSMO/MESSy is zero or undefined outside of the coupled region, i.e., the horizontal and vertical relaxation areas as well as those parts of the globe which are not covered by the COSMO/MESSy instance. Therefore, the uncovered points are filled with the ozone field calculated by EMAC, as for the calculation of the radiative flux in EMAC, global, non-zero fields must be fed into the diagnostic routine. With this ozone field a second, diagnostic radiation call is performed using RAD. Two simulations are investigated:

- **REF**: EMAC and COSMO/MESSy are using the same emission data set (MACCIty, Granier et al., 2011).
- SENS: EMAC uses the MACCIty inventory, while COSMO/MESSy applies a DLR specific inventory.

Here, the difference of the radiative fluxes ('COSMO/MESSy minus EMAC'), area averaged over Central Europe ($35^{\circ}:60^{\circ}$ N; $-10^{\circ}:30^{\circ}$ E) for July 2008 are compared. Figure 7a shows the vertical profiles of the differences of the clear-sky radiative fluxes applying the same emissions (REF). The larger ozone values as simulated by COSMO/MESSy compared to EMAC near the tropopause lead to a positive radiative flux difference in the longwave as well as in the shortwave bands around 200 hPa. If the emissions in COSMO/MESSy are changed (SENS, Fig. 7b), lower ozone values are simulated by COSMO/MESSy compared to EMAC up to around 800 hPa. These lower values lead to a negative difference of the longwave radiative fluxes compared to EMAC.

4.3 2-way coupling of prognostic variables

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20 Next, we show two examples for the coupling of 3D-3-D prognostic variables. First, the 2-way coupling of dust tracers between EMAC and one COSMO/MESSy instance is shown. Secondly, all dynamical variables of two COSMO/MESSy instances are coupled 2-way to demonstrate the potential of the 2-way coupling. To avoid the adjustment of the topographies, the smaller COSMO/MESSy instance is predominantely located over the ocean.

4.3.1 **Dust**

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Dust emissions are very sensitive to the model resolution, as they depend on the soil type and the wind velocity. Typically, dust emission schemes are developed for a specific model resolution and include scaling factors to adapt the emission scheme to other resolutions as good well as possible.

In our example, we use a MECO(1) setup, coupling the dust tracers of a COSMO/MESSy instance with 0.36° horizontal resolution back to the EMAC model in T63 spectral resolution.

Figure 8 shows the dust emission fluxes integrated over a domain ranging from 60°W to 60°E and from 45°S to 45°N. Due to different soil type distributions and higher wind maxima in the COSMO/MESSy instance, the latter produces much higher dust emission fluxes, as the simulation was performed without any scaling of the emissions resolution dependent optimisation of the emission scheme. These higher emissions are reflected also in the horizontal dust column mass (mg/m²) distribution. Figure 9 displays the dust column mass for March 06, 2004. Panel A shows the dust column mass (in mg/m²) in the COSMO/MESSy instance, panel B the EMAC dust column mass in the 1-way coupled simulation, and panel C the result of the 2-way coupled simulation. Obviously, the COSMO/MESSy instance exhibits much finer structures as both EMAC instances. However, the maximum present in the COSMO/MESSy instance is much better represented in the EMAC 2-way simulation, as intended.

This simulation contains still a small error with respect to the vertical distribution of the dust, as the height adjustment for the topography orography is not yet consistent for the two coupling directions (see above). Nevertheless, this examples illustrates the potential of the 2-way coupling to improve the coarse representation of quantities, which are determined by smaller scale features.

4.3.2 Hurricanes

Tropical cyclones (TCs), developing at the West coast of Africa over the tropical East Atlantic, are known to be precursors for hurricanes causing damages in the US (e.g., Ike, 2008; Dean, 2009) or over Europe (e.g., Helene, 2006; Katia, 2011). Those TCs often originate as disturbances of the African Jet Stream, so-called African Easterly Waves (AEWs) over the African continent. In case of suitable conditions over the Atlantic, these AEWs have the potential to develop into TCs and finally to hurricanes. Therefore, forecasting the development, track and intensity of hurricanes requires both, a high model resolution to capture all the multi-scale interactions, prerequisite for the development of the initial TC, and a huge model domain capturing the African continent as well as the Atlantic ocean (e.g., Rappaport et al., 2009; Schwendike and Jones, 2010).

As an example, the development of a hurricane named ISAAC is analysed here. It originated in September 2000 as a TC from an AEW at the West coast of Africa. The National Hurricane Center classified it as a hurricane for the first time on 23 September 12 UTC, before it reached maximum intensity as a category 4 hurricane on 28 September 18 UTC (https://coast.noaa.gov/hurricanes/). Afterwards, its track turned to the north-east and after extratropical transition the system reached Great Britain readily identifable by strong wind gusts two days later.

To demonstrate the potential of the dynamical 2-way coupling between two COSMO/MESSy instances, a MECO(2) set-up is applied to simulate the development of ISAAC. This means, two COSMO/MESSy instances, varying in horizontal resolution,

time step length and model domain, are nested into coupled to the global EMAC model. While the finer resolved $(0.11^{\circ} \approx 12 \text{ km})$ COSMO/MESSy instance is driven by the coarser resolved $(0.22^{\circ} \approx 25 \text{ km})$ COSMO/MESSy instance, initial and boundary data for the coarser COSMO/MESSy instance are transformed from EMAC (T106 $\approx 120 \text{ km}$). Since this study focuses on the specific development of ISAAC, a weak nudging of four prognostic variables (temperature, divergence, vorticity and the logarithm of surface pressure) towards ECMWF analysis data is applied for EMAC (as described by Jöckel, 2006) during the first two weeks after start of the simulation (15 September 0 UTC). Once the hurricane leaves the model domain of the finer resolved COSMO/MESSy instance (29 September 0 UTC, Fig. 11) the nudging is switched off and the EMAC instance is completely unconstrained afterwards. In case the COSMO/MESSy instances are coupled 2-way, the dynamical information from the finer resolved instance, comprising the temperature (T), the wind velocities (U, V, W), pressure perturbation the pressure deviation from the reference atmosphere (PP) and moisture (QV, QC, QI) are fed back to the coarser instance. The domains covered by the model instances are shown in Fig. 11 (grey and blue areas).

In Fig. 10 and 11 the results obtained with 2-way coupled COSMO/MESSy instances (right panels) are compared to those of the one-way coupled system (left panels). Deviations are validated using the HURDAT data set (Landsea and Franklin, 2013), which is part of the International Best Track Archive for Climate Stewardship (IBTrACS (v03r04), Knapp et al., 2010, available at http://atms.unca.edu/ibtracs/ibtracs_v03r04/browse-ibtracs/).

Although EMAC is nudged during the genesis phase, the development of ISAAC is not captured by EMAC, as there is no pressure decrease visible in the time series of minimum sea level pressure (SLP_{min}, Fig. 10, black contour). In contrast, ISAAC initially originates in both COSMO/MESSy instances (Fig. 10, blue and red contours), independent of the coupling strategy and horizontal resolution and approximately at the correct time (23 September) compared to the best track estimate (Fig. 10, green contour). However, there are strong differences comparing the one-way and 2-way coupled instances during the ongoing development of SLP_{min}: while the final intensification of ISAAC simulated with the one-way coupled instances does not start before 26 September, the 2-way coupled instances are able to capture the initial decrease. Even though the intensity of ISAAC in the one-way coupled simulations coincides better with the reference on 27 September, the position and further track of ISAAC differs distinctly from the best track position (Fig. 11) from this time on. In contrast, the dynamical 2-way coupling between the COSMO/MESSy instances leads to a correct representation of the track and intensity of ISAAC in the coarser resolved model instance, even after the system has left the model domain of the finer resolved instance.

By simulating the development of ISAAC with the MECO(2) set-up, the potential of the dynamical 2-way coupling between two COMSO/MESSy instances is demonstrated: to capture the multi-scale interactions, prerequisite for the development of the initial TC of ISAAC, in this case a horizontal model resolution of 0.11° is required. The model domain of this fine resolved instance, however, can be kept small, if the dynamical information are fed back to the coarser resolved model instance in the 2-way coupled mode.

Overall, the results of the examples shown here, indicate that the 2-way coupling has the potential to improve the representation of hurricanes in the coarser COSMO/MESSy model instance.

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5 Model Performance

Due to technical reasons, the frequency of data exchange between the child and the parent model must be the same as for the parent-to-child data transfer. During the latter, the two slices of the boundary fields, for which COSMO performs a linear time interpolation, are filled with the data of the actual time step. This was required to enable a non-sequential 2-way coupling. However, it limits the choice of the coupling frequency, which should be chosen as small as possible, i.e., as the smallest common multiple of the parent and the child model time step. For this reason, a sensitivity analysis of different coupling frequencies is not provided here.

Usually people are aware of other couplings (e.g. ocean-atmosphere coupling) in which, for instance for mass conservation, fluxes need to be accumulated / averaged over the coupling interval. In contrast to this, our 2-way coupling of two atmosphere models utilises a relaxation technique at the lateral boundaries for the parent-to-child exchange, and within the entire coupling domain for the feedback from child to parent, thus modifying the model results according to the finer resolved fields. Thus, since we do not couple fluxes for which mass conservation would be required, but correct the results directly, accumulation or averaging aver time is not feasible.

The run-time performance depends first and foremost on the specific model setups (e.g. on the complexity of the chosen chemistry representation etc.). But most important, the overall performance is at the end determined by the "degree of balance" of the distribution of parallel tasks among the different model instances. We discussed this in detail in part II of our series (Kerkweg and Jöckel, 2012b) for the 1-way nesting case. The same principles hold for the 2-way exchange, except for the complication that communication waiting times depend now on bi-directional data exchange. Thus, it is up to the user to find (experimentally) the optimum task distribution to minimise communication waiting times.

Fig. 12 sketches exemplarily the costs of the coupling. A MECO(2) setup similar to the hurricane case, was integrated for 1 day and the residence time in the respective routines transforming the data has been measured. Because the child model does all the data transformations between the two grids, it consumes much more computing time than the parent model. The difference between the one-way coupled (black) and the solely dynamically 2-way coupled (red) simulation is small, as only six additional fields need to be interpolated. Already for the one-way coupled simulation, adding 139 chemical tracers (black dashed line) triples the processing time in the child model, while it requires the sixfold time, if they are 2-way coupled (red bashed line).

In contrast to this, the number of coupling fields provokes no systematic increase of computing time in the parent model.

Although the coupling time increases significantly in the child model, the time consumption for the coupling is still negligible in comparison to the computing time required for the calculation of the chemistry of these 139 chemical tracers.

6 Conclusions

In this article we present the next generation of the Multi-Model-Driver (MMD v2.0). While MMD (v1.0) provided all tools required for the 1-way coupling of dynamical and chemical models (e.g., EMAC and an arbitrary number of COSMO/MESSy

instances) following a client-server approach, version v2.0 was further developed to allow for data exchange from the client to the server model.

To reach this goal, the MMD library was expanded by the respective subroutines for the data exchange via MPI. The new submodel MMD2WAY includes the features of the previous MMD (v1.0) submodels MMDCLNT and MMDSERV plus all functionalities for the data transfer from the child to the parent model.

The new MESSy infrastructure submodel GRID is used for the transformation from the child model grid to the subpart of the parent model grid overlapped by the child model. For the horizontal grid transformation data remapping the SCRIP software implemented in the GRID submodel is used, while. For the vertical regridding procedes by the usage of for COSMO-EMAC coupling NREGRID, which is also part of the GRID submodel, is utilised. In contrast to this, the vertical remapping for the COSMO-COSMO coupling is performed using the spline-interpolation as provided by INT2COSMO.

Currently, an inconsistency between the vertical regridding routines in <a href="https://example.com/https

The capabilities of the 2-way coupling has been demonstrated on the basis of four examples: (a) a comparison of fields upscaled from the regional model to the global model grid with the global model fields, (b) the comparison of radiative forcing calculated consistently with the same radiation scheme, (c) the 2-way coupling of dust tracers, which emission fluxes are highly grid resolution dependent, and (d) the dynamical coupling of two COSMO/MESSy instances influencing the development of a hurricane within the coarse COSMO/MESSy model domain.

The Supplement contains the manuals for the MESSy infrastructure submodel GRID, for the MMD library and the MMD User Manual. Additionally, a more detailed list of the setups of the example simulations is provided in the Supplement.

To develop a fully dynamical 2-way coupling for the MECO(n) system, the https://example.com/interactions routines need to be replaced by more generic routines to enable a fully consistent coupling in both directions.

Code availability. The code as described is part of the Modular Earth Submodel System (MESSy), which is continuously further developed and applied by a consortium of institutions. The usage of MESSy and access to the source code is licenced to all affliates of institutions which are members of the MESSy Consortium. Institutions can be a member of the MESSy Consortium by signing the MESSy Memorandum of Understanding. More information can be found on the MESSy Consortium Website (www.messy-interface.org). The submodel GRID and the 2-way coupling code are part of the official MESSy distribution (code release v2.53 and younger).

Author contributions. A. Kerkweg was the leader of the FLAGSHIP project. She developed the largest part of MMD (library and MMD2WAY submodel) and the generic submodel GRID. Ch. Hofmann and G. Pante have been part of the FLAGSHIP project and considerably contributed to the MMD2WAY development. Ch. Hofmann performed the hurricane study. G. Pante provided the results of the dust tracer example. M. Mertens was the first "FLAGSHIP external user" of the 2-way coupled system and contributed the radiative forcing example.

P. Jöckel was one of the master minds of the FLAGSHIP team. Additionally, the GRID software is based on the NCREGRID software developed by him. Thus he considerably contributed to the implementation of the GRID submodel.

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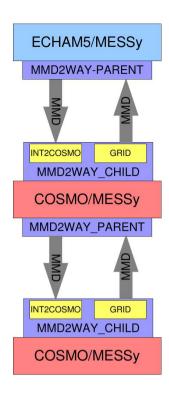


Figure 1. Illustration of the connection between the different MMD parts. The example is for a MECO(2) setup, i.e., EMAC with a cascade of 2 nested COSMO/MESSy instances.

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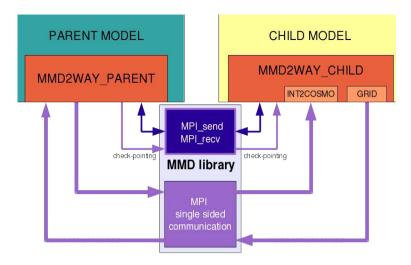


Figure 2. Illustration of the communication managed by MMD between a parent and a child model. Dark violet colours indicate data flow during the initial phase, while purple indicates the data flow during the integration phase.

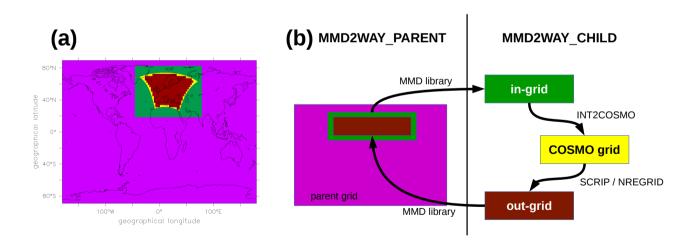


Figure 3. Relation of the different grids: EMAC grid in pink, the in-grid and out-grid defined by MMD2WAY_CHILD in green and brown, respectively, and the COSMO/MESSy model grid in yellow. Panel A(a): position of the different grids relative to each other, for the example of a European domain; Panel B:(b) illustration of data flow between the different grids.

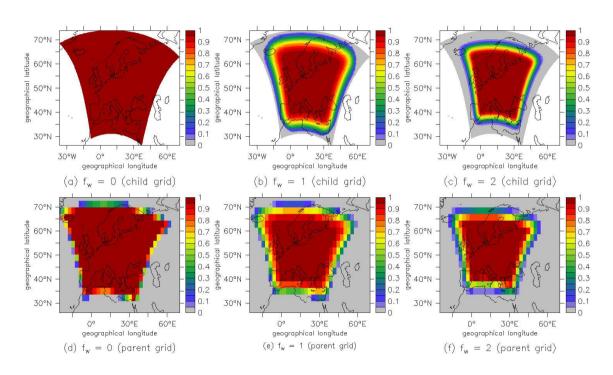


Figure 4. Weight functions (f_w , see Sect. 2.2, page 9) for the different weight types. Upper row: weight functions as calculated on the child model grid. Lower row: weight functions after transformation to the parent model grid.

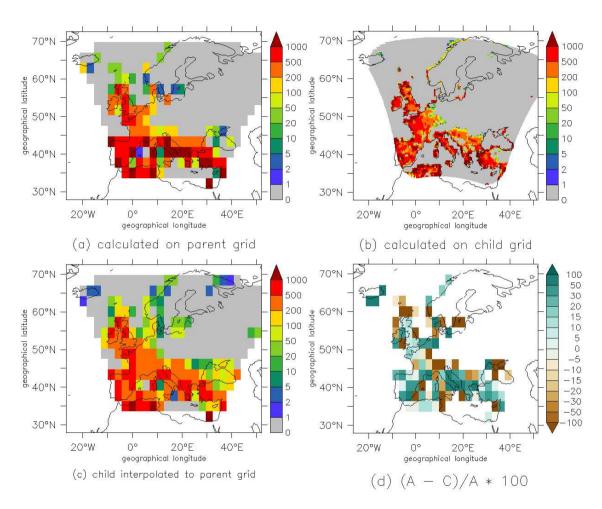


Figure 5. Biogenic NO emissions flux in $pg \ m^{-2} \ s^{-1}$ for one distinct date in January 2003. The data has been mask masked to show only the coupled region.

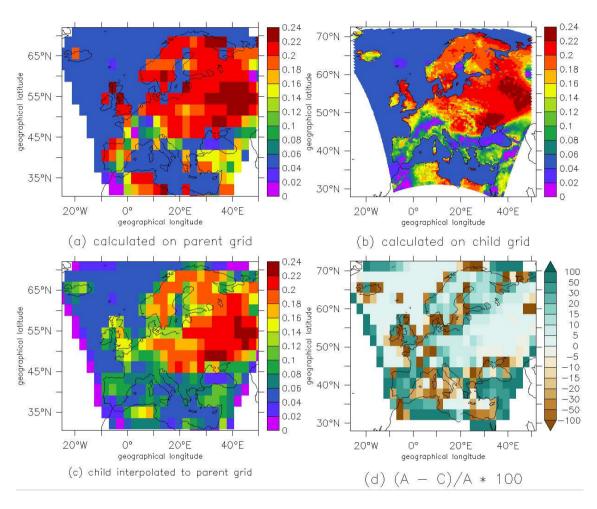


Figure 6. Ozone dry deposition velocities in $cm\ s^{-1}$ for one distinct date in January 2003. The data has been $\frac{mask\ masked}{mask\ masked}$ to show only the coupled region.

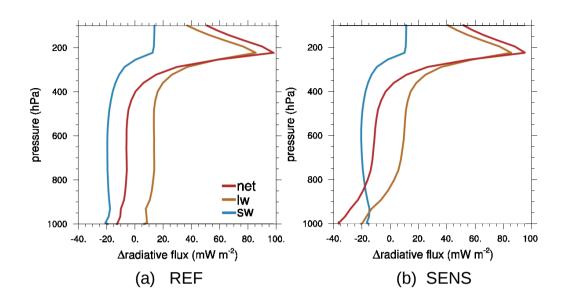


Figure 7. Differences ('COSMO/MESSy minus EMAC') of the radiative fluxes (shortwave (sw), longwave (lw) and net) averaged over 35° N - 60° N and -10° E - 30° E for July 2008. (a) REF simulation; (b) SENS simulation.

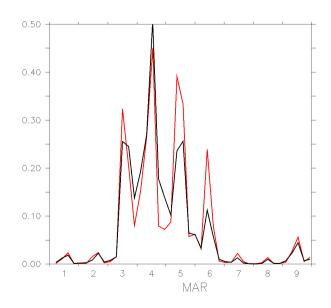


Figure 8. Time series of dust emission (Gg) in the EMAC (black) and in the COSMO/MESSy (red) instance.

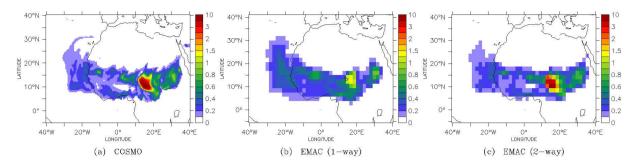


Figure 9. Dust column mass (mg m^2). Shown is an instantaneous value for March 06, 2004, 00 UTC. Left panel: for COSMO/MESSy; middle panel: for EMAC; right panel: for 2-way coupled EMAC, thus influenced by the COSMO/MESSy instance.

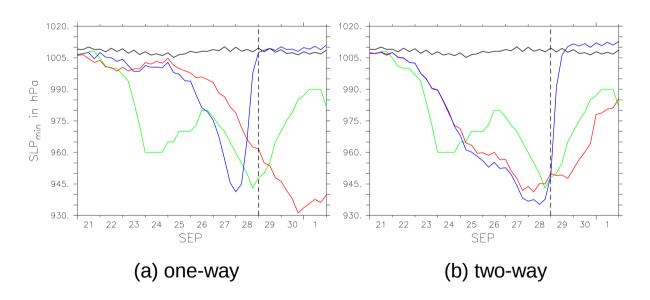


Figure 10. Time series of SLP_{min} (in the area of 10°N - 50°N and 65°W - 25°W) in the one-way (left) and 2-way (right) coupled simulation for EMAC (black), COSMO/MESSy_{0.22} (red), COSMO/MESSy_{0.11} (blue) based on 6-hourly data. The best-track intensity from HURDAT is shown as reference (green). EMAC is nuged until 29 September (dashed line, s. text for details).

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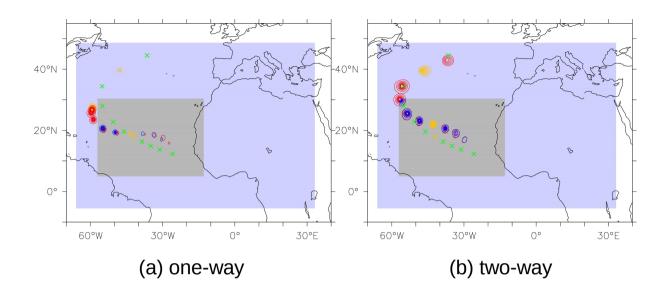


Figure 11. Track position for hurricane ISAAC in the one-way (left) and 2-way (right) coupled simulation. The daily SLP (less than 1005 hPa, 5 hPa-intervalls, in the area of 0°N - 50°N and 65°W - 25°W, starting on 23 September 0 UTC) is shown as contours for the COSMO/MESSy instances (red: COSMO/MESSy_{0.22}, blue: COSMO/MESSy_{0.11}). The best-track position from HURDAT is marked as reference (green crosses). To allow for a temporal comparison, the positions on 26 September and 1 October are yellow coloured for all tracks. The different model domains of the COSMO/MESSy instances are shaded (blue: COSMO/MESSy_{0.22}, grey: COSMO/MESSy_{0.11}).

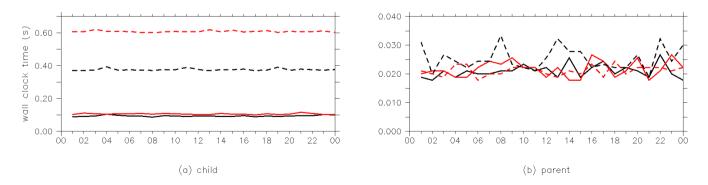


Figure 12. Hourly averaged wall clock time spent for the processing of the coupling data in the submodels (a) MMD2WAY_CHILD and (b) MMD2WAY_PARENT for a MECO(2) setup, shown for different couplings between the two COSMO/MESSy instances: one-way coupling (black), 2-way dynamical coupling (red). The dashed lines are for the additional coupling of 139 tracers.