Supplementary material

A. Kerkweg et al.

This document is available as electronic supplement of our article "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)" in Geosci. Model Dev. (2018), available at: `http://www.geosci-model-dev.net`

Impact of orography differences on the vertical profile

Interpolating back and forth between differently resolved orography 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. S1 displays at four different locations, the height profiles of the tracer in the parent domain, 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. For this specific case parent model and child model initial profiles are identical, indicating that the tracer is initialised with exactly the same height profile in both COSMO instances. With increasing surface height difference, the differences in the vertical profiles increase. The second row of Fig. S1 displays the differences of the blue and the red line, i.e., of the original profile and the profile given by the coupling field.

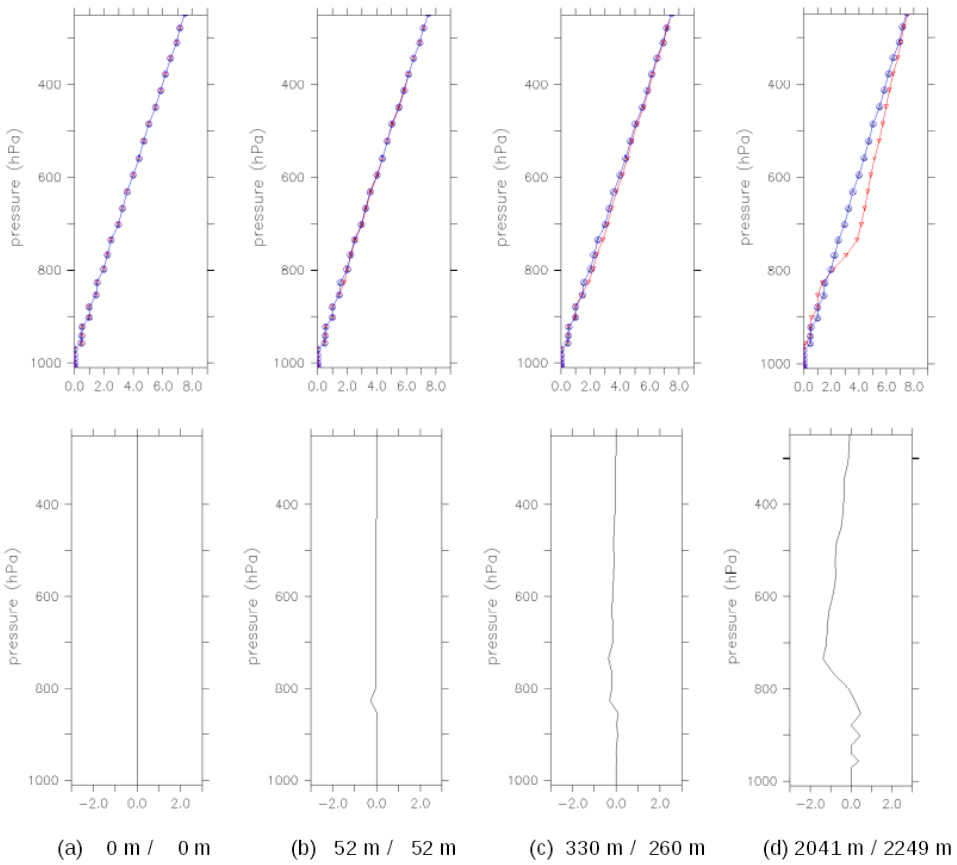

Figure S1: Vertical profiles of a passive tracer (upper row) and its differences (lower row) for different topographic heights in the two COSMO/MESSy model instances (in $10^{-10} mol/mol$). The title indicates the topographic height in the parent / child domain, respectively. Blue line (circles): initial profile in the child model and in the parent model; red line (topdown triangles): coupled tracer profile in the parent model. The lower row displays the differences between the blue and the red lines.

Example:
Performance of 2-way nesting for one specific setup

The run-time performance depends very much on the chosen setup. The largest impacts are

- the complexity of the simulation itself (e.g., whether or not chemistry is included),
- the number of coupled fields,
- the sizes of the coupled domains,
- the number of chosen tasks, and
- the task distribution between the different model instances.

Thus, all numbers that might be shown here, are only valid for exactly the one specific setup as analysed in the example. We apprehend that these numbers might be misleading and could be wrongly interpreted. Therefore we are hesitating to show such numbers in the main body of the article. However, as a compromise, we include the analysis given below in the supplement, and add a reference to it in Sect. 5.

Table 1 shows the run time in node hours for a 1 day simulation of one specific MECO(2) setup, applied with four different task distributions (S01-S04) on 3 nodes (à 24 tasks) at the Mistral computer at Deutsches Klimarechenzentrum (DKRZ). For the mere dynamical setups S02 is the fastest, as could be expected from the number of horizontal grid boxes in CM1 and CM2 and the fact that only the child model has to perform the data transformations. This is still the case for the 1-way simulations including 139 tracers. However, the additional time required for the 2-way coupling is largest in the case with 139 tracers for this setup (45.3%). This shows that the required additional time for the 2-way nesting is extremly setup dependent. Thus, the best task distribution needs to be chosen by the user for each setup individually. Here, the user has to take into account at least the size of the different model domains, the number of 1-way and / or 2-way coupled variables, and the complexity of the simulation, e.g. whether or not chemistry is included.

On the first glance the required additional time seems to be large. However, the tracers in this example are only transported. No chemical kinetic calculations are included. Including chemistry, at least 10 times higher run times are to be expected. Thus the additional run time for the 2-way nesting would shrink dramatically relative to the overall run time of chemical applications.

Name	Configuration	DYN		139 Tracer	
	EMAC - CM1 - CM2	1-way	2-way	1-way	2-way
S01	6x1 - 5x6 - 6x6	0.488	0.512 (4.9%)	1.520	2.120 (39.5%)
S02	6x1 - 4x6 - 7x6	0.468	0.480 (2.6%)	1.500	2.180 (45.3%)
S03	6x1 - 3x6 - 8x6	0.494	0.532 (7.7%)	1.580	2.240 (41.8%)
S04	6x1 - 2x6 - 9x6	0.524	0.530 (1.1%)	1.680	2.320 (38.1%)

Table 1: Node hours required for a 1-day simulations with a MECO(2) setup employing EMAC in T42L31ECMWF, COSMO/MESSy with 120x120 horizontal grid points, 40 levels, and COSMO/MESSy 91x91 horizontal grid points, 40 levels. The "configuration" column denotes the task distribution between EMAC, the first COSMO/MESSy instance (CM1) and the second COSMO/MESSy instance (CM2). The right most 4 columns list the run time in node hours for a mere dynamical setup (DYN, 1-way vs. 2-way nested) and a setup including 139 1-way and 2-way nested tracers (but without chemical kinetics). Additionally, the column for the 2-way applications provide the additional run time required for the 2-way nesting in percent. The simulations have been performed at the "mistral" computer system at the German Climate Computing Center. The node hours are taken from the scheduler output.