



Supplement of

An enhanced emission module for the PALM model system 23.10 with application for PM₁₀ emission from urban domestic heating

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S1. Preamble

This document serves as a rudimentary guide for compiling the PALM model system source code variant developed for the accompanied paper and provides instructions for running the cases listed in §§ 3.3 and 4. Both the source code and the accompanying run cases can be retrieved under DOI 10.5281/zenodo.10890465.

It is expected that the user has first-hand experience handling large-scale computational models at a source code level in a Unix/Linux operating environment. These include but not limited to console-based file and system operations, building the PALM model system and all dependencies from source, launching model runs in parallel through MPI, as well as scheduling jobs to a computational cluster via a workload manager such as TORQUE and Slurm.

S2. Building PALM model system from source

First, the user should download the PALM model system 23.10 from the Gitlab page below:

```
https://gitlab.palm-model.org/releases/palm_model_system/
releases/v23.10
```

and follow the instruction on the page below for installation and configuration:

```
https://gitlab.palm-model.org/releases/palm_model_system
```

For convenience, the root directory of the PALM model system will be referred to as `palm_model_system/` throughout this document.

Once the model system has been successfully set up, download the source code and the test cases from the DOI indicated in the preamble and extract the contents of the `".tar.gz"` archive to a separate directory. It consists of two directories:

- `src/` : This directory contains the exact state of the PALM model system source code that has been used for creating all contents featured in this article. To use this PALM model system source code, replace the contents of the directory `palm_model_system/packages/palm/model/src` with the files contained in this `src/` directory. Backing up the original source directory before replacement is highly recommended.
- `JOBS/` : This directory contains input data for the performance benchmark cases for this article (performance*), as well as the idealized domestic emissions test case (idealized_domestic). They should be copied to the directory `palm_model_system/packages/palm/model/build/JOBS`.

The PALM model system can now be rebuilt using the command `palmbuild`. Any dependency requirements not yet satisfied, for instance, for netCDF, fftw, and RRTMG, will be reported by `palmbuild` at this time. The onus is on the user to resolve them.

S3. Launching model runs

With a successful build, each of the performance benchmark and the idealized domestic emissions test case can then be run.

Each model run (under `palm_model_system/packages/palm/model/build/JOBS`) contains a directory called `INPUT`, which contains all necessary input data, as its name suggests. At a minimum, it consists of a model parameter namelist (the `_p3d` file) as well as a netCDF file containing all surface information (the `_static` file).

An additional file can also be found for the idealized domestic emissions test case to facilitate job resubmission (the `_p3dr` file) in the likely event that the run reaches the maximum allocated runtime before the end of the model run is reached.

Depending on hardware resources, the jobs can be launched locally and interactively or submitted to a computational queue using the command `palmrun`. The following is a recommended setting for the model runs:

```
palmrun -B -v -r [case name] ...  
        -X 400 -T 50 -a "d3# restart" -b -t 43200
```

where `[case name]` refers to the corresponding model run presiding in the PALM model system `JOBS` directory.

Note that the `palmrun` arguments `-X` and `-T` specify the total number of compute cores and the number of compute cores per compute node respectively. Meanwhile, the argument `-t` specifies the maximum allowable time for which the model run in question can be conducted on the HPC, in this case 12 hours, or 43200 seconds. The `restart` option is used for cases that require resubmission (i.e., beyond the period specified by the `-t` argument), such as the idealized domestic emissions test case; it should be omitted if the job is not expected to continue through resubmission.

Upon completion of each run, the user should be able to locate two additional folders on each model directory (located under `palm_model_system/packages/palm/model/build/JOBS`):

MONITORING/ : This directory contains all forms of diagnostic information accumulated during the model run.

OUTPUT/ : This directory contains the model output in netCDF format.

Further information on PALM input and output files can be found in the following link:

<https://palm.muk.uni-hannover.de/trac/wiki/doc/io>