Project: **677**

Project title: **Evaluierung der Atmosphärenchemie in MECO(n)**

(for 2024 changed to **Model development and support for the MESSy system (FZJ-IEK-8 part)**

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Report period: **2022-11-01 to 2023-10-31**

Maximum of 2 pages including figures. 9 pt minimum font size.

The application for 2023 the planned work was subdivided into five subprojects:

1. Further implementation of MESSy chemical submodels into ICON/MESSy and Tests
2. Reimplementation of MESSy into ICON via the library ComIn.
3. Test of GPU ported code on Levante
4. Development of an ICON-CLM/MESSy package for COPAT2
5. (Part of) the User Support for MESSy

As stated in the request for 2023, this project is a pure model development and user support project for issues arising around the further development of the MESSy software. This has two consequences: (1) the amount of required computing time and /work storage space is highly speculative, as it depends on the arising debugging requirements. (2) the range and the prioritising of the work to be done is rapidly changing. One example is, that due to the success of the natESM support sprint for developing a MESSy infrastructure component which allows minimise the copies between host and device in a partly ported setup, most of the actual development work was done to adapt the MESSy code to the needs arising by such an infrastructure component.

This accounting period the support requests were not that computing time demanding as expected in our application and, due to the shift to the GPU developments, the development took much more human working time than computing time for testing. This is why we did not use most of the computing time applied for in the reporting period.

1. <u>Further implementation of MESSy chemical submodels into ICON/MESSy and Tests</u>
   The following MESSy process submodels have been ported and tested to be usable in ICON/MESSy in 2023:
   - AIRSEA (air-sea exchange of trace gases)
   - LNOx (lightning NOx)
   - MSBM (calculation of heterogenous reaction rates in the upper atmosphere)
   - O3ORIG (diagnostic for O3 origin)
   - PTRACINI (artificial initialisation of passive tracers)
   - QBO (QBO nudging)
   - VERTEX (calculation of important transfer coefficients in the lowermiost atmospheric layer)
2. <u>Reimplementation of MESSy into ICON via the library ComIn.</u>
   The ComIn natESM sprint is ongoing. However, only a marginal amount of computing time was used from the computing project for some a priori tests.
3. <u>Test of GPU ported code on Levante</u>
   The natESM sprint for GPU porting run from January until May 2023. No computing time was used for the developments by the programmer (Enrico Gregori) of the natESM sprint himself, as he used the DKRZ budget. However, at the end of the sprint we had a concept and an implementation of the infrastructure expansion to enable an efficient management of the data copies between the devices.
   To fully implement the newly developed concept, interface routines are required to be established or strictly used instead of direct data usage to ensure that the new

infrastructure component can log all data usages / copies between devices. The further development and update of all MESSy submodels was the largest part of development and test work performed within this computing project.

4. <u>Development of an ICON-CLM/MESSy package for COPAT2</u>
As there was no demand from the CLM-Community side to use the MESSy extensions for the evaluation of ICON-CLM this project was postponed. In future this special development would anyhow be replacable by using the ComIn interface with MESSy as third-party model.

5. <u>(Part of) the User Support for MESSy</u>
A number of User Support requests / bug reports have been processed.
Explaining these in detail would go beyond the scope of this report, but they could be checked in the MESSy GitLab at DKRZ.