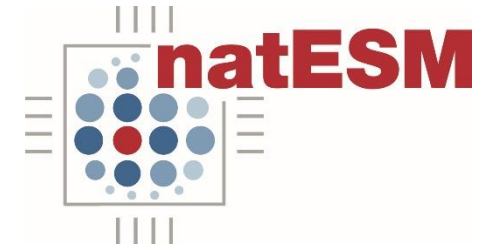


Workshop – natESM strategy

21. February 2022, virtual meeting

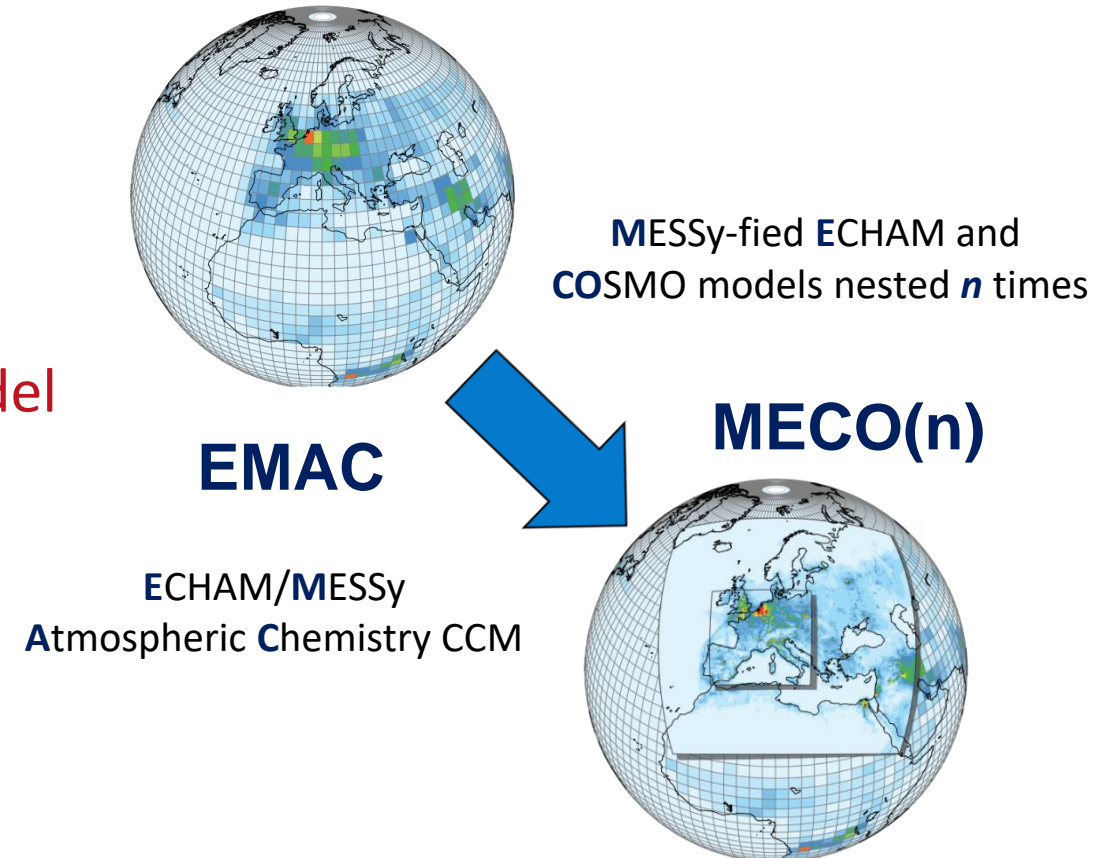


Request for support sprint

Implement YAXT¹ as standard library for all MPI communication in MESSy (Modular Earth Submodel System) (simulation)

Deutsches Zentrum für Luft- und Raumfahrt e.V. (DLR)
Contact: Kerstin Hartung

1: Yet Another eXchange Tool

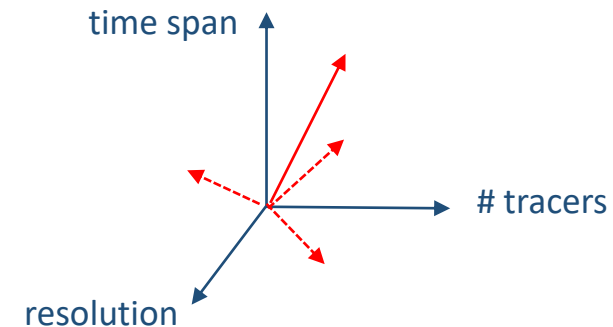


© Mariano Mertens (DLR)

The natESM support team is located at DKRZ and JSC. Based on a DKK initiative of the German Earth System Modelling Community, the overall goal is to build a national ESM strategy for the future.

Brief Overview of Model/Software

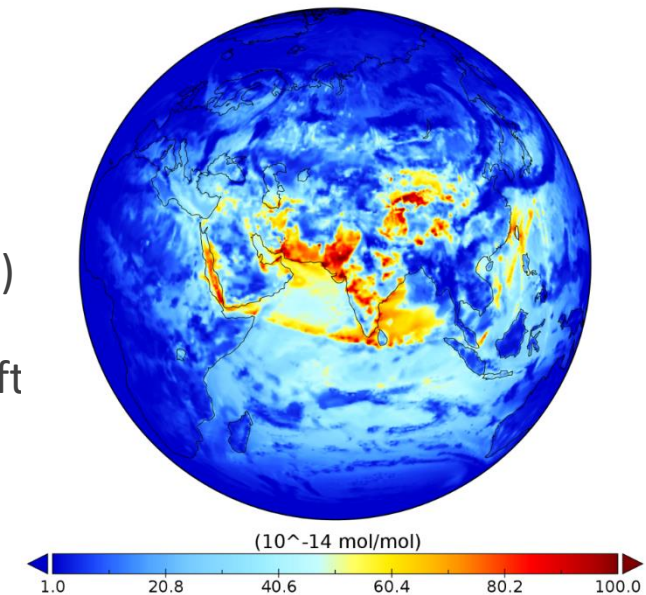
- ESM field: global and regional **chemistry climate** and **air quality** modelling
- User group: large consortium of 12 German and 12 international institutions, around **220 users** and 40 submodel and 5 infrastructure developers
- Targeted simulations:
 - **complex chemical simulations** to idealized simulations
 - on **local, regional and global spatial scales**
 - over various **timescales**
- HPC usage:
 - MPI-based parallel domain decomposition
 - running at DKRZ, JSC, LRZ, MPCDF, SARA (NL) etc.
- Maintenance:
 - **MESSy code parts are open source**, the basemodels (ECHAM, ICON, COSMO) are license limited
 - the source code is hosted on the DKRZ GitLab server
 - all consortium members contribute to the **documentation** and development of MESSy
 - every 1-2 years a new “tagged” version is released



Model/Software Application Field

- Scientific highlights: 474 publications on and with MESSy since 2005
 - estimating the contribution of traffic emissions to tropospheric ozone (Mertens et al., 2020)
 - modelling the impact of COVID-19 emission reductions on tropospheric ozone (Mertens et al., 2021)
 - studies as part of the Chemistry Climate Model Intercomparison (CCMI) projects (e.g. Jöckel et al., 2016)
- Social relevance:
 - contributions to WMO/UNEP Ozone assessment report (CCMI) and IPCC (CMIP)
 - used for health and hazard studies (e.g. Chowdhury et al., 2021)
 - impact of anthropogenic emissions on air quality and climate (e.g. DLR, TU Delft and NLR).
- Plans for further use and dissemination:
 - transition to ICON as basemodel
 - open source as much as possible
 - develop model for improved air quality and chemistry climate research

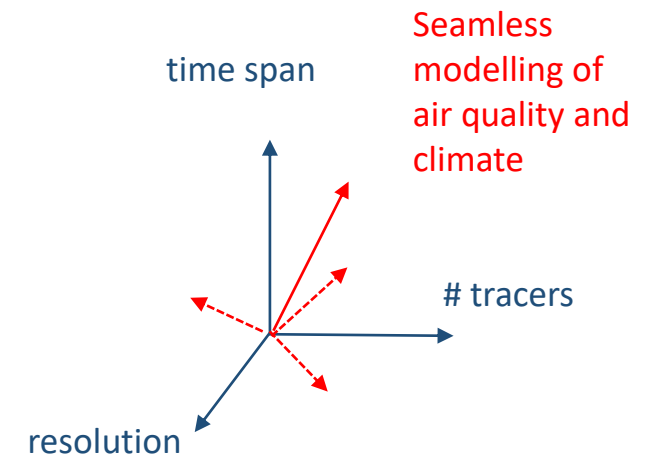
Hydroxyl (OH) at ground level



T255L31, 60 km / 0.5°
Domenico Taraborrelli (FZJ)

Description of Planned Work

- Scope of Request:
 - communication via YAXT instead of current basemodel-specific MPI calls, implementation in new MESSy infrastructure submodel which translates MESSy internal data structures to YAXT decompositions
 - 6 month duration
 - **available on HPC systems** on which MESSy is currently used
- Criteria for fulfilment: specific MPI calls superseded by **YAXT-based communication, in generic subroutine** but activated for at least one basemodel
- Expected scientific and/or performance improvements:
 - increased **performance portability** due to use of YAXT
 - **more modular** internal parallel communication; facilitating updates, expansion and exchange by other parallelisation models
 - alternative parallelisation strategies can be more easily tested
 - basis for efficient and clean expansion to scalable optimized I/O, which is a requirement for future HPC architectures
 - allow for **finer resolved simulations over longer timescales or in ensembles**



References

- Chowdhury, S., Haines, A., Klingmueller, K., Kumar, V., Pozzer, A., Venkataraman, C., Witt, C., & Lelieveld, J.: Global and national assessment of the incidence of asthma in children and adolescents from major sources of ambient NO₂, Environmental Research Letters, doi: 10.1088/1748-9326/abe909, URL <https://doi.org/10.1088/1748-9326/abe909>, 2021.
- Jöckel, P., Tost, H., Pozzer, A., Kunze, M., Kirner, O., Brenninkmeijer, C. A. M., Brinkop, S., Cai, D. S., Dyroff, C., Eckstein, J., Frank, F., Garny, H., Gottschaldt, K.-D., Graf, P., Grewe, V., Kerkweg, A., Kern, B., Matthes, S., Mertens, M., Meul, S., Neumaier, M., Nützel, M., Oberländer-Hayn, S., Ruhnke, R., Runde, T., Sander, R., Scharffe, D., & Zahn, A.: Earth System Chemistry integrated Modelling (ESCiMo) with the Modular Earth Submodel System (MESSy) version 2.51, Geoscientific Model Development, 9, 1153–1200, doi: 10.5194/gmd-9-1153-2016, URL <http://www.geosci-model-dev.net/9/1153/2016/>, 2016.
- Mertens, M., Kerkweg, A., Grewe, V., Jöckel, P., and Sausen, R.: Attributing ozone and its precursors to land transport emissions in Europe and Germany, Atmos. Chem. Phys., 20, 7843–7873, <https://doi.org/10.5194/acp-20-7843-2020>, 2020.
- Mertens, M., Jöckel, P., Matthes, S., Nützel, M., Grewe, V., and Sausen, R.: COVID-19 induced lower-tropospheric ozone changes, Environ. Res. Lett., 16, <https://doi.org/10.1088/1748-9326/abf191>, 2021.