natESM Community Workshop 2024

27.-28.02.2024 ▪ Marriott Hotel ▪ Am Hallischen Tor 1 ▪ 04109 Leipzig

Breakout Group:
Atmospheric Chemistry and Aerosol Component

Ina Tegen, TROPOS. - itegen@tropos.de

Talks:

- Florian Prill (DWD) - ComIn
- Patrick Jöckel (DLR) ICON-MESSY via ComIn
- Ali Hoshyaripour (KIT) ICON-ART
- Bernd Heinold (TROPOS) ICON-HAM
- Jens Stoll (TROPOS) ICON-MUSCAT

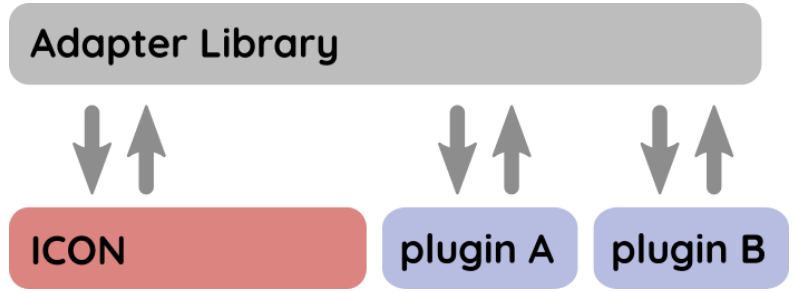
Briefly introduce the model or software, short and long-term plans for model development, particularly with regard to the use of the ComIn coupler.

ComIn – Florian Prill, DWD

Project started 2022 as a collaboration between **DWD**, **DLR-IPA** and **DKRZ**

The community interface

- connects 3rd party modules to the ICON host model
- plugin functions are called at pre-defined events
- regulates the access and creation of model variables



Shared libraries for Fortran or C/C++ plugins.

Python plugins do not need any compilation process at all.

Roadmap for v0.2.0 - Upcoming features:

- development tool **comin_replay -** *test ComIn plugins with previously recorded data sets*
- GPU host-device transfer
- combining ComIn with YAC - *ComIn is an interface, not a translation layer*
- generalizations: additional meta-data; edge-based and vertex-based fields, ...

Summary & Outlook

- MESSy is an easily expandable, highly flexible, open software framework, which was originally designed for atmospheric chemistry research
- applications: box-models on chemical kinetics, regional air-quality, (chemistry) forecasts for measurement campaigns, chemistry-climate interactions, …
- all scales; vertical range from boundary layer to upper atmosphere
- includes a wealth of on-line diagnostics
- all SMs described on wep-page: https://www.messy-interface.org
- 42 Phd theses and ~ 500 peer reviewed publications so far

- transition from ICON/MESSy to ICON-ComIn/MESSy (see talk by K. Hartung on natESM sprint)
- fit for GPUs (work in progress, see talk by A. Kerkweg on natESM sprint)
- (!) MESSy open source
- continuous further development within (open) consortium

  Note: each shown submodel (=process implementation) can easily be complemented by alternatives (e.g. we do already have 2 comprehensive aerosol schemes sharing the framework)

  → attractive to bring your own code into it
- potential natESM users: everything related to chemistry in the Earth System

ICON-ART
Ali Hoshyaripour, KIT

1. ART is a component of the ICON code with shared. infrastructure (e.g. CI) and governance.
2. ICON-ART is used by DWD in several operational applications including weather forecasting
3. The interface is developed to ensure modularity and flexibility
4. Open source code released alongside ICON code in Jan/24
5. The model system can be configured for LES to global studies of aerosols and chemistry.
6. Website, Wiki, tests and documentation are available to support the used community
7. The main ongoing efforts focus on GPU porting, coupling with ICON-Seamless and process acceleration with ML.

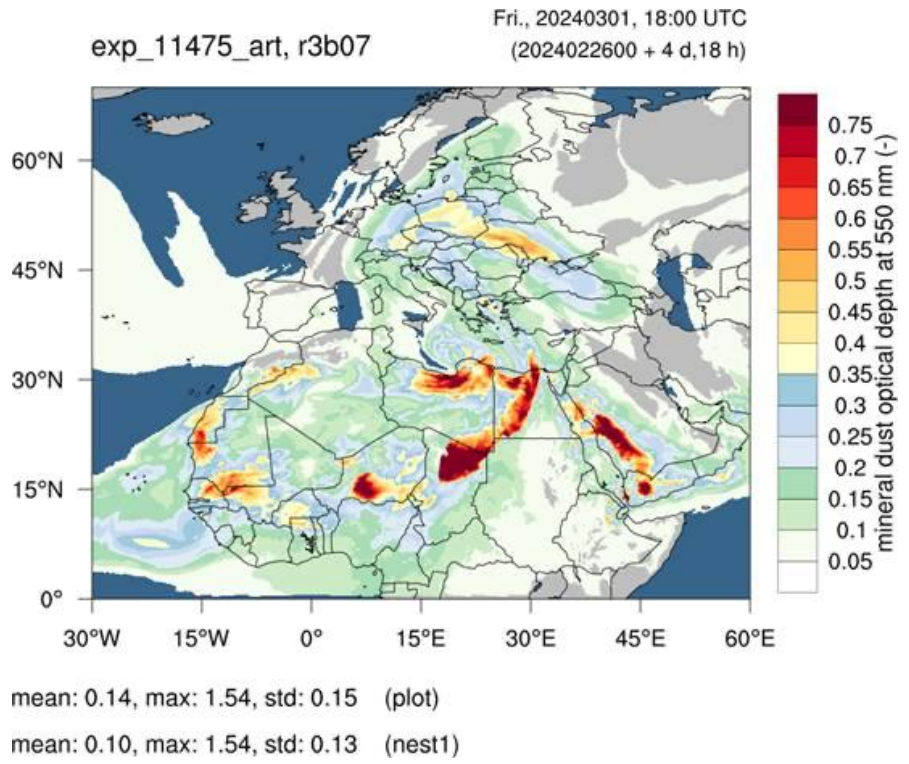


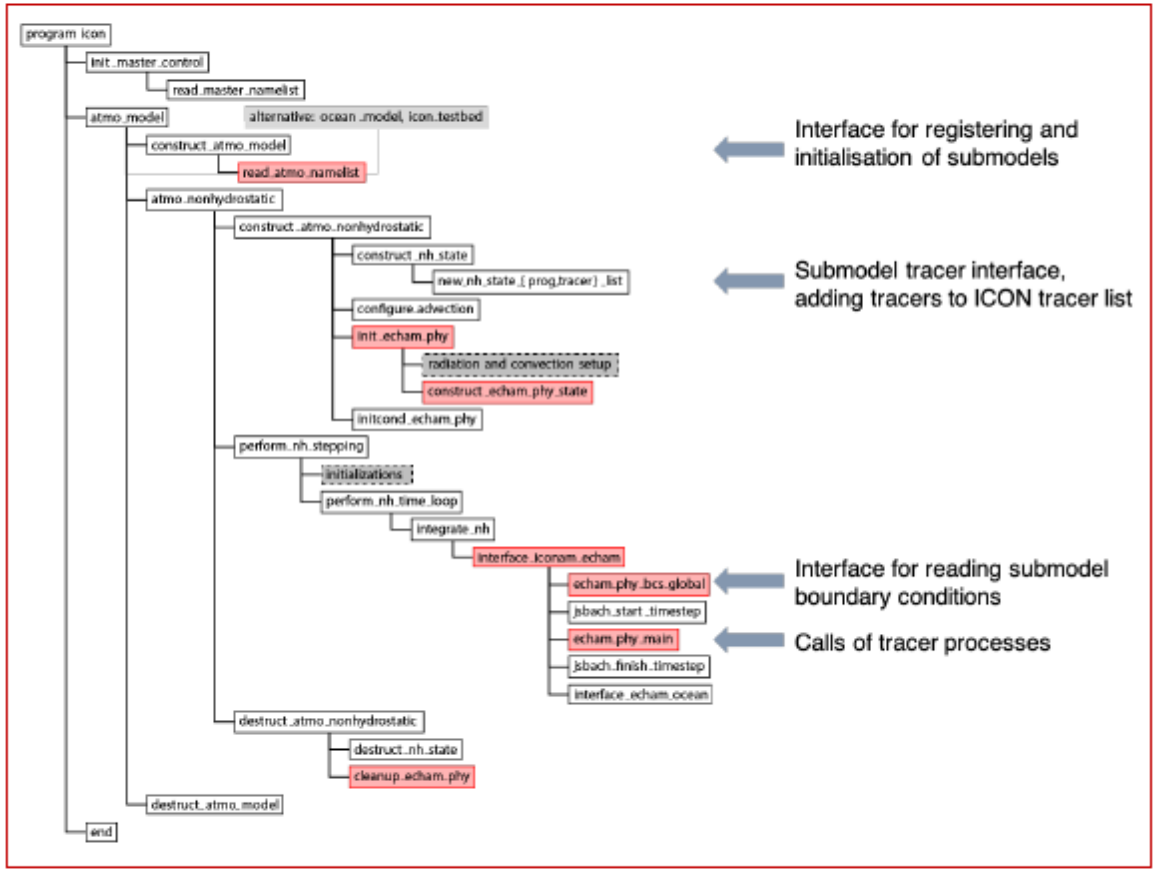
Figure: *Prediction of mineral dust AOD from ICOM ART for 01.03.2024*

ICON-HAM coupling

Bernd Heinold, TROPOS

- Following the HAMMOZ submodel interface concept:
  - Minimal changes to host model (no changes to parameter lists, no submodel-specific code nor names)
  - Modularisation with submodels registering to host model / being triggered by master switch, own submodel namelists
- Using ICON infrastructure for I/O, etc.
- Separate file structure and compiler directives
- *./configure --enable-jsbach --with-hammoz*
- ICON Community Interface will simplify the coupling but does not yet fully support it, as entry points are currently outside the "block loop"

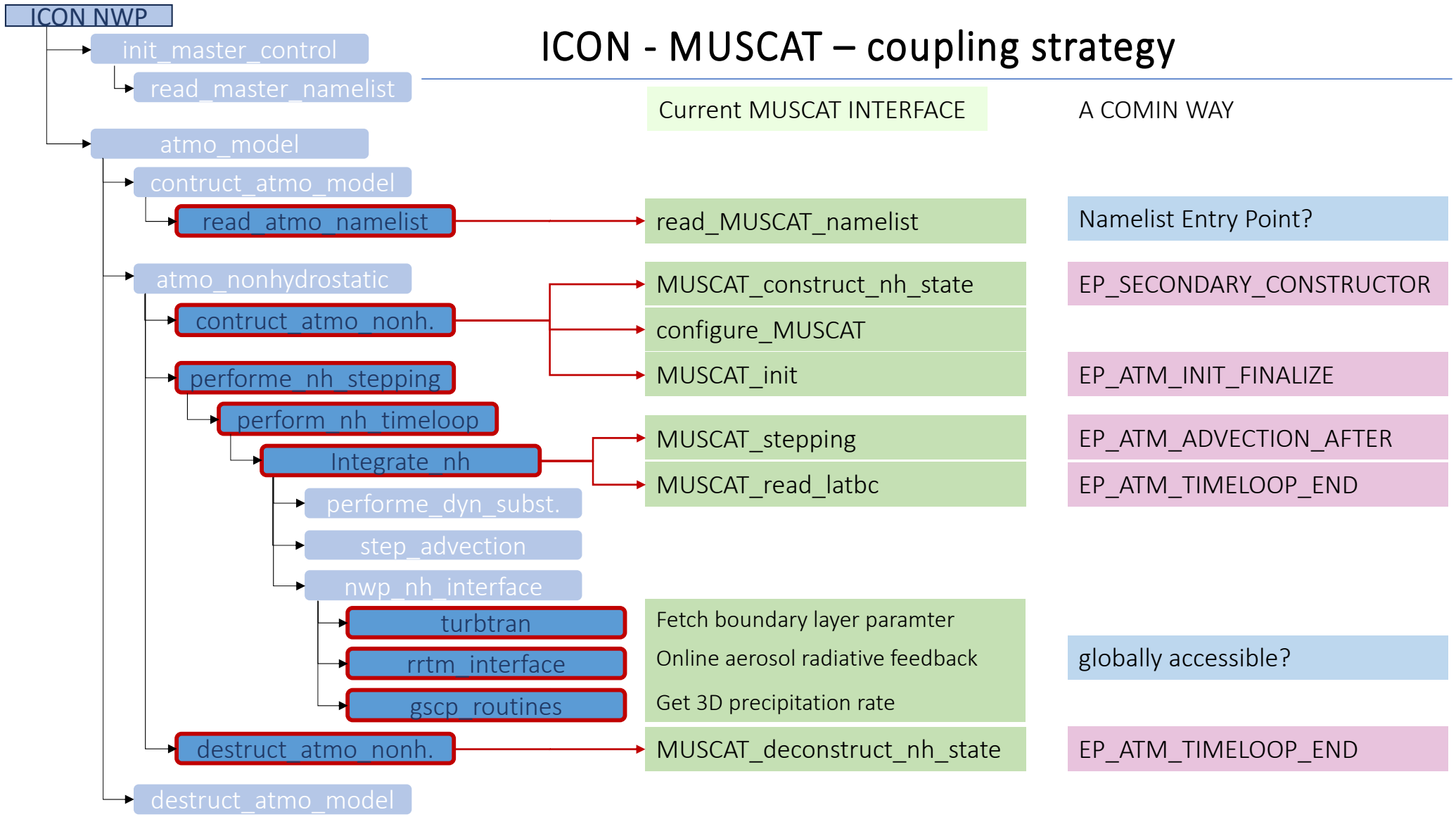
Model coupling flowchart



Salzmann et al., JAMES, 2022

Jens Stoll, TROPOS

ICON - MUSCAT – coupling strategy



Discussion:

1. Leading question: Would it be useful for the German research community to endorse one or several aerosol/chemistry model(s) as NatESM core component(s)? Would this actually be a feasible option?
2. ~~Should aerosol/chemistry modelling be treated as optional component in the NatESM?~~
3. ComIn is viewed as an extremely useful tool for coupling aerosol/chemistry models to ICON and its role as important core infrastructure for NatESM is unquestionable.
4. Supporting single aerosol/chemistry model as part of NatESM would reduce needs of duplicates or triplicates of same tasks to be carried out for different models. Also this would be the version to be used for CMIP experiments
5. Are model groups willing to modify their own strategy to work toward a single atmospheric/chemistry component version of NatESM?

Discussion (cont.):

6. Three German aerosol/chemistry models fulfil (nearly) all technical requirements for NatESM components, while having different target user groups
7. There may be need for an additional/refined list of requirements for an aerosol/chemistry component
8. Suggestion to revive the ICON Atmopheric Composition working group (established 2018, DLR, FZ Jülich, KIT, DWD, TROPOS, MPI-C) as a NatESM working group, reassess their recommendations and establish a specific model criteria list.