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Coupling MESSy via ComIn to ICON: a status report

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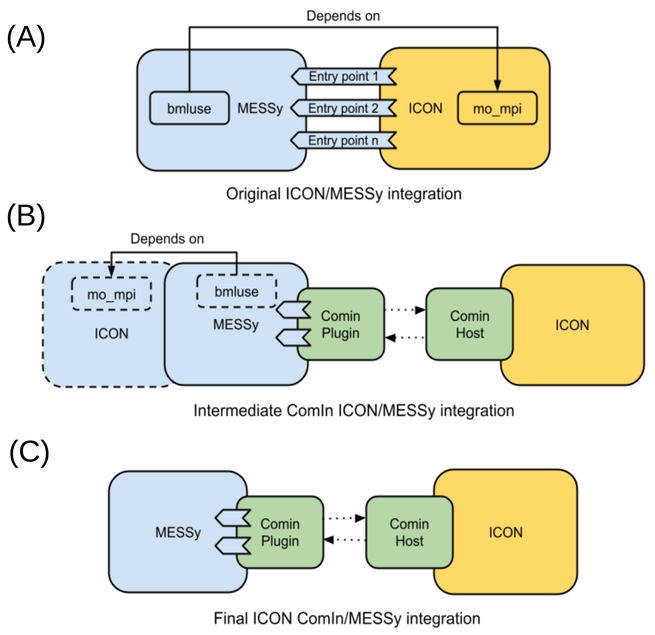
Abstract:

The Community Interface (ComIn, **(A)**) was developed to provide a stable interface for integrating a variety of third-party models, so-called plugins, into the ICON model. A number of relatively simple examples and test plugins are provided with ComIn, but a comprehensive evaluation of its capabilities is still pending. In particular, we want to demonstrate the successful coupling of a complex model to ICON via ComIn.

The Modular Earth Submodel System (MESSy, **(B)**) is a rather complex model as it is mainly used for simulations of atmospheric chemistry. For applications with complex atmospheric chemistry, the computational effort is more than 10 times higher than for a purely dynamic ICON simulation. Efficient coupling through ComIn is crucial here.

Supported by two natESM sprints (www.nat-esm.de), the integration of MESSy into ICON via ComIn is not yet complete. We will provide an overview of the required changes (compared to the hardwired integrated ICON/MESSy version) and give an update on the current status of the coupling.

Development steps from ICON/MESSy to ComIn/MESSy



The figure on the left displays the different development stages of ICON/MESSy.

Panel (A) depicts the starting point. MESSy is attached to ICON via subroutine coupling: at different locations in the ICON code the so-called MESSy entry points are called from hooks in the ICON code. Additionally, the MPI communication, the descriptive data (p_patch) etc. are directly USEd from ICON.

Panel (B) visualises the intermediate state created during the first natESM ComIn sprint. This configuration was constructed to enable the developers of the ComIn to replace the hard-coded ICON↔MESSy exchange piece-wise by ComIn exchange while keeping the possibility to check the individual steps in a version of the code, which is compiling and running.

Panel (C) pictures the final state of MESSy being attached to the ICON code as a ComIn plugin. MESSy entry points are called via ComIn call-backs. Required ICON data are provided solely by ComIn. No direct access of ICON data / interaction between MESSy and ICON takes place.

(A) ComIn

ICON **Com**munity **In**terface
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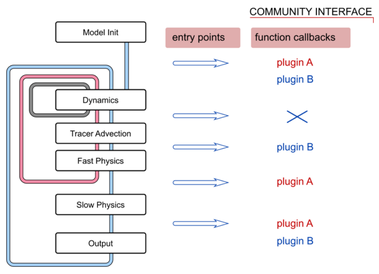
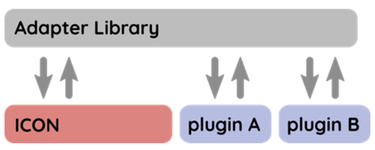
What are the aims of ComIn?

- ➡ Providing a standardized **public interface** for third party codes (‘**plugins**’) coupled to ICON
- ➡ Significantly **reduced maintenance** for ICON as well as for third party code developers
- ➡ Plugins **easier to migrate** to new ICON releases
- ➡ Establishing ICON as the core model for applications ranging from **NWP** to **ESM**
- ➡ Enables **multi-language support** (Fortran, C/C++, Python)

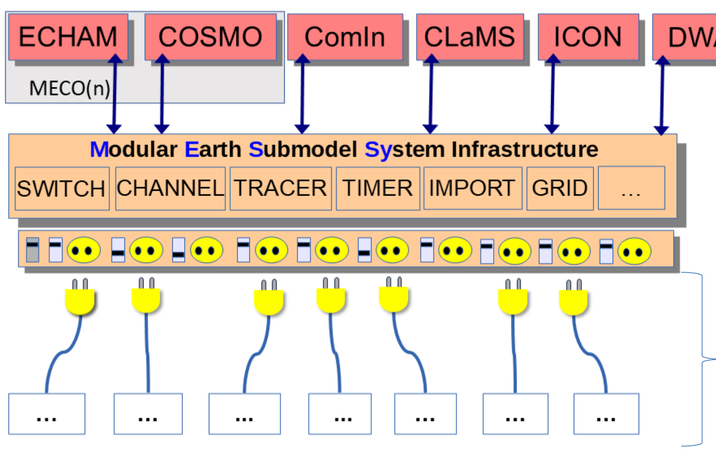




How does ComIn work in a nutshell?

- ➡ ComIn organizes the **data exchange** and **simulation events** between the ICON model and multiple plugins.
- ➡ **ComIn Callback Register**: Subroutines of the plugins are called at pre-defined events during the ICON simulation.
- ➡ The **ComIn Adapter Library** is included by ICON and the plugins. It contains descriptive data structures and regulates the access and the creation of model variables.

(B) The Modular Earth Submodel System (MESSy)



(licency) **base models**

infrastructure
connecting different type of base models (grids, decomposition, …) with base model independent MESSy submodels

sub-model = process descrip-tion

submodel interface
connect submodel core (= scientific content) to infrastructure

submodel core
base model independent: diagnostics, physical or chemical process in basic entity (e.g. box for a kinetic solver, column for convection

MESSy was mainly developed to provide a flexible framework for all kinds of chemistry climate and air quality applications.

MESSy provides a middleware for coupling atmospheric legacy models (e.g., ICON, ECHAM, COSMO) and specialized ESM components, the so-called submodels (e.g., physical parameterizations, chemistry packages, diagnostics) via generalized interfaces for standardized control and coupling. Currently more than 100 submodels are included in MESSy.

ICON global variables

Pointers to the global ICON variables (i.e., those listed in variable lists of ICON) are exposed via ComIn.

To enable access for the MESSy submodels, those are made available as MESSy channel objects.

1. To define the representation (dimensions of the objects on all active ranks) correctly, the dimensions of the different ranks and their role (ncells, nvert, nproma, nlev…) need to be clear
   a) loop over all exposed variable, create channel objects, where representation could be deduced from the currently available information; √ done
   b) Implementation of dimension semantics in ICON and its exposure in ComIn required; work in progress (WIP)
   c) use new dimension semantics for channel object generation; waiting for 1b)
2. Implement update of channel object memory pointer for multi-timelevel variables during the time loop. √ done
3. As intermediate test option: implement parallel output via pnetcdf. √ done

TIME synchronisation

MESSy has its own time management routines (TIMER). This needs to become synchronised with the ICON date and time settings:

1. The models start and stop date are exposed via ComIn and the TIMER dates can be set accordingly. √ done
2. The time steps of the individual domains are exposed by ComIn as well and can be applied in MESSy TIMER. √ done

CHECKPOINTING / RESTART

Currently, **ComIn does not expose any restart information**. What is exposed and when in the timeloop is still under discussion!

Up to now, …

1. MESSy sets up regular check-pointing and restart intervals (TIMER namelist). This could be achieved by
   a) either ensure that the run-script sets the same intervals in the ICON and the TIMER namelist
   b) or by exposing additionally the check-pointing / restart dates and intervals via ComIn.
2. MESSy is able to trigger a restart (QTIMER/TIMER namelists) or extra check-pointing (TIMER namelist)
   - only available solution is the usage of ICONs utility-file-hack “lstop_on_demand”

With ComIn, ICON now is the only master of check-pointing and restarting and ICON also schedules restarts or check-pointing outside of the namelist determined regular intervals. This information needs to be exposed early enough to MESSy and other plugins to enable them to prepare their data for check-pointing.

ongoing discussion

TRACER

Even though tracers belong also to the global variables of ICON, they are treated differently in MESSy.
ComIn exposes always a pointer to the 5-D tracer memory of the current time level.
This is used as “new time level” in TENDENCY, while the array for the value at the end of the previous time step (now) is allocated by MESSy and filled with a copy of the new time level at the end of the time step.
Necessary steps for the tracer implementation are:

1. Expand MESSy to deal with one time slice of the tracer memory being externally provided. √ done
2. Implement update of tracer channel objects after change of ComIn pointer target during the time loop. √ done
3. Modify TENDENCY to directly integrate tracers, instead of storing all tendencies in a tendency field and perform the final integration at the end of the time step. √ done
4. Access and apply MESSy-tracer tendencies for convection and turbulence, which are calculated but not applied in ICON and exposed via ComIn. (WIP)
5. Advective tendency diagnostic (TENDENCY) (WIP)

MPI - parallel communications

So far, MESSy always used the MPI implementation of its respective base model. This is no longer possible with ComIn. ComIn exposes those data required to establish the required communication patterns in the plugin itself.
This entails a complete restructuring of the MESSy MPI submodel: The new MPI submodel needs to provide the communication routines all by itself. We distinguish basically two ways of communication

1. those communications (e.g., broadcasts), which only require the models’s communicator (does not have to be MPI_COMM_WORLD) √ done (some cleanup required)
2. transpositions (as gather and scatter), requiring information about the parallelisation and the data. For this the YAXT library is used. (WIP)

Note: The establishment of a MESSy MPI submodel and MESSy's own parallel communication functions is the important step to get from the intermediate state (B in figure at top) with a kind of ‘backpack ICON’ to the final state (C), in which all ICON data is only transmitted via ComIn.

Additional data / things required for ICON

to be started when TRACER, MPI and RESTARTs are finished

- the maximum number of tracers in ICON is currently 1600. In its final application state, MESSy will define up to 9000 tracer.
- MESSy creates “END” file, if simulation is aborted => use **comin_callback_context_call** in subroutine **abort_mpi.**
- In several places access to local fields is required:
  - TERRA: wet skin fraction **zf_wi**
  - Microphysics scheme:
    - large scale precipitation cloud cover [0-1]
    - large scale rain precipitation flux [kg/(m^{2}s)]
    - large scale snow precipitation flux [kg/(m^{2}s)]
    - large scale rain precipitation flux without cloud production of new rain [kg/(m^{2}s)]
    - large scale snow precipitation flux without cloud production of new snow [kg/(m^{2}s)]
    - rain formation rate [kg/kg], averaged over box
    - snow/ice formation rate [kg/kg], averaged over box
    - large scale frozen precipitation melting [kg/kg]
    - large scale ice sedimentation [kg/kg]
  - Convection scheme
    - convective cloud water content (3d in cloud) [kg/kg]
    - convective cloud ice content (3d in cloud) [kg/kg]
    - convective precipitation formation (water, in cloud) [kg/kg]
    - convective precipitation formation (snow, in cloud) [kg/kg]
    - convective entrainment rate in upward flux [kg/(m^{3}s)]
    - convective entrainment rate in downward flux [kg/(m^{3}s)]
- microphysics: in PSC regions, the microphysics calculations need to be replaced (overwritten?) by the calculations of the MESSy submodel MSBM

Literature:

- Hartung, K., Kern, B., Dreier, N.-A., Geisbüsch, J., Haghighatnasab, M., Jöckel, P., Kerkweg, A., Loch, W. J., Prill, F., and Rieger, D.: ICON ComIn – The ICON Community Interface (ComIn version 0.1.0, with ICON version 2024.01-01), Geosci. Model Dev. Discuss., https://doi.org/10.5194/gmd-2024-135, in review, 2024.
- Jöckel, P., Kerkweg, A., Pozzer, A., Sander, R., Tost, H., Riede, H., Baumgaertner, A., Gromov, S., and Kern, B.: Development cycle 2 of the Modular Earth Submodel System (MESSy2), Geosci. Model Dev., 3, 717–752, https://doi.org/10.5194/gmd-3-717-2010, 2010