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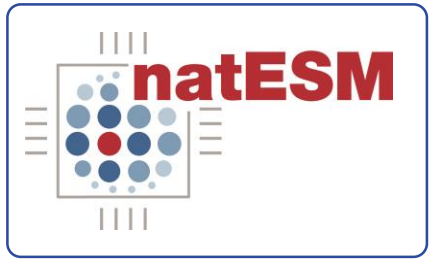
Wetter und Klima aus einer Hand

Generic concepts of ICON ComIn

F. Prill & ICON ComIn project team



DWD, DLR, DKRZ | natESM Tech Training | Hamburg | 17 July 2024

Intro: Plugin mechanism for ICON

Demo script that runs alongside the ICON simulation:

```python
import comin
import numpy as np

comin.var_request_add(("my_var", 1), False)

@comin.register_callback(
  comin.EP_SECONDARY_CONSTRUCTOR)
def simple_python_constructor():
    global pres, my_var
    print("simple_python_constructor called!")
    pres = comin.var_get(
      [comin.EP_ATM_WRITE_OUTPUT_BEFORE],
      ("pres", 1))
    my_var = comin.var_get(
      [comin.EP_ATM_WRITE_OUTPUT_BEFORE],
      ("my_var", 1))
```

```python
@comin.register_callback(
  comin.EP_ATM_WRITE_OUTPUT_BEFORE)
def simple_python_diagfct():
    np.asarray(my_var)[:] = 42.

@comin.register_callback(comin.EP_DESTRUCTOR)
def simple_python_destructor():
    print("simple_python_destructor called!")
```

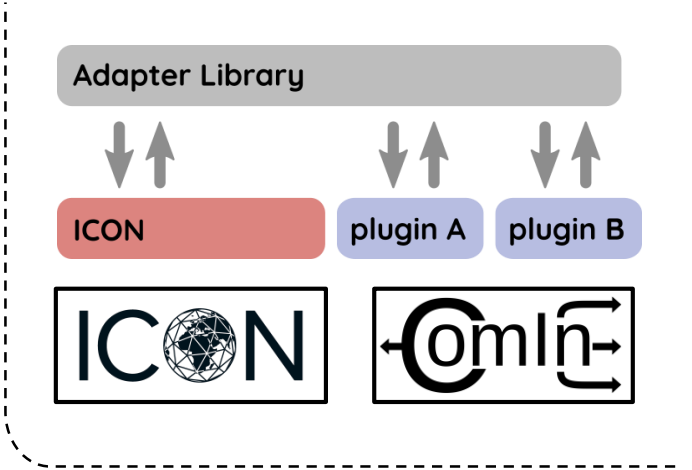
ComIn = ICON Community Interface

The community interface

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

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

Python plugins run without compilation process.



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

ComIn is part of the Open Source Release of ICON 2024.01 [1].

Note: Similar solutions exist for the NOAA models or the IFS [2].

[1] https://gitlab.dkrz.de/icon/icon-model
[2] IFS Plume: https://github.com/ecmwf/plume

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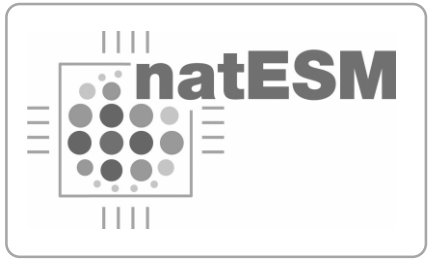
Running an existing plugin



Plugging into ICON's control flow

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About 40 **entry points**

- Ex.: **`EP_ATM_WRITE_OUTPUT_BEFORE`**

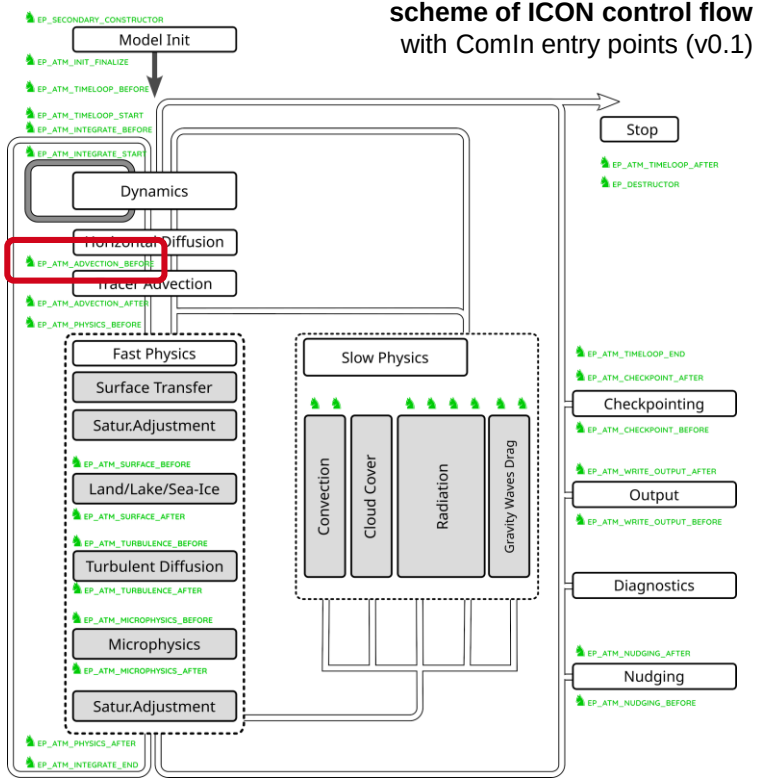
  "before/after" nomenclature
  `EP_<COMP>_<PROCESS|LOOP>_`↵
  `[BEFORE|AFTER|START|END]`

- ICON host model: look out for
  `CALL icon_call_callback(…)`

ComIn entry points

- dependent on namelist settings and program flow
- preliminary and easily expandable! Feedback welcome!

scheme of ICON control flow
with ComIn entry points (v0.1)



How to enable ICON ComIn

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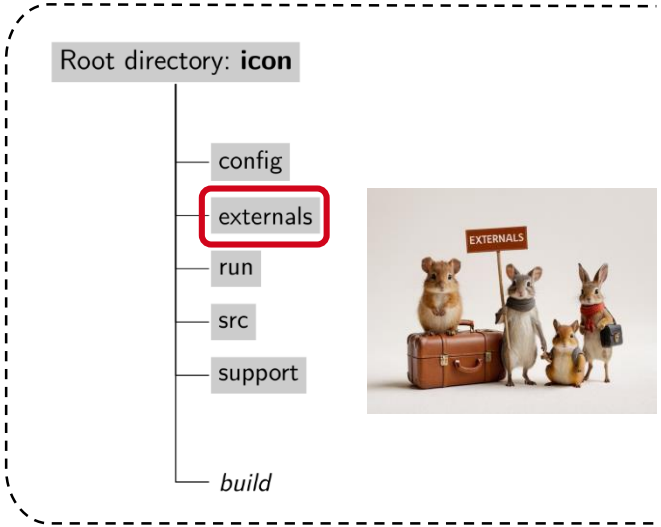
ComIn is a switchable external ICON package contained in the ICON release https://gitlab.dkrz.de/icon/icon-model.

```
../config/dkrz/levante.gcc --enable-comin
```

- Alternatively, you can download a standalone version. ComIn releases published independently from ICON [1].
- The Python adapter itself is implemented as a ComIn plugin written in C++. It comes together with the ComIn library and embeds the Python interpreter.



User guide, technical description ... https://icon-comin.gitlab-pages.dkrz.de/comin

[1] https://gitlab.dkrz.de/icon-comin/comin/-/releases

`configure --enable-comin` … and then what?

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Register your plugin in the host model via namelist.

ICON

multiple plugins can be attached

```
&comin_nml
  plugin_list(1)%name           = "comin_plugin"
  plugin_list(1)%plugin_library = "libpython_adapter.so"
  plugin_list(1)%options        = "comin_plugin.py"
/
```

filename of the Python script is passed as an option

Optional: non-standard name of constructor, MPI communicator, user-specified plugin arguments (character string)

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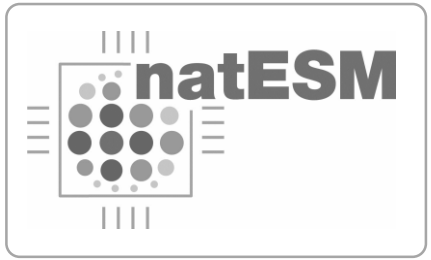
Developing a plugin



primary constructor / callback function(s) / descriptive data structures / variable access

Building blocks ... Primary constructor

Primary constructor: registers the plugin and additional variables.

- Note: In Fortran or C/C++ plugins, the primary constructor is a separate subroutine; for Python this is simply the main body.
- API functions are exposed in the Python module `comin`, needs to be imported.

```
import comin
var_descriptor = ("comin_process_id", jg)
comin.var_request_add(var_descriptor, lmodexclusive=False)
comin.metadata_set(var_descriptor, zaxis_id = comin.COMIN_ZAXIS_2D)
```

variables are identified by name + domain ID

main purpose of the primary constructor: request additional variables

Building blocks ... Secondary constructor

By the term secondary constructor we denote an entry point at the end of ICON's initialization. That's the first time when you can obtain readable and writable pointers to the ICON data fields.

this tells ComIn about the context, ie. the entry point where we use the variable

```
myvar = comin.var_get([comin.EP_ATM_WRITE_OUTPUT_BEFORE],
                      ("comin_process_id", jg),
                      flag=comin.COMIN_FLAG_WRITE)
```

this is a variable handle! see next slide.

again, ComIn identifies variables by name + domain ID

Descriptive data structures contain information on the ICON setup and the simulation:

```
domain = comin.descrdata_get_domain(jg)
clon = np.asarray(domain.cells.clon)
```

Building blocks ... Callback function(s)

Callbacks for specific entry points are realized as custom Python functions.

- registered with ComIn by adding a function decorator
- note: the secondary constructor is a callback like any other

function decorator with entry point ID

```
@comin.register_callback(comin.EP_ATM_WRITE_OUTPUT_BEFORE)
def simple_python_callbackfct():
    myvar_array = np.asarray(myvar)
```

variable handle from the previous slide

Access to the variable data is provided via NumPy/CuPy objects.

Building blocks: Summary


```
import comin
import numpy as np
```

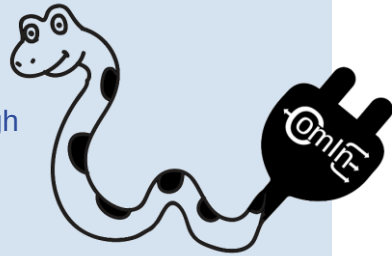
primary constructor:
request additional ICON variable

```
comin.var_request_add(("my_var", 1), False)
```

```
@comin.register_callback(↵
  comin.EP_SECONDARY_CONSTRUCTOR)
def simple_python_constructor():
    global pres, my_var
    print("simple_python_constructor called!")
    pres = comin.var_get(
      [comin.EP_ATM_WRITE_OUTPUT_BEFORE],
      ("pres", 1))
    my_var = comin.var_get(
      [comin.EP_ATM_WRITE_OUTPUT_BEFORE],
      ("my_var", 1))
```

secondary constructor: get variable handles

callbacks: register function callbacks through Python decorators




```
@comin.register_callback(↵
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def simple_python_diagfct():
    np.asarray(my_var)[:] = 42.
```

```
@comin.register_callback(comin.EP_DESTRUCTOR)
def simple_python_destructor():
    print("simple_python_destructor called!")
```

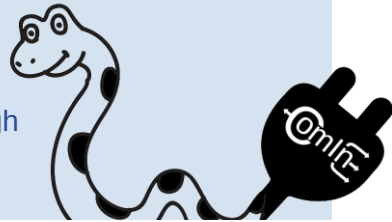
See the ComIn release code for more demo plugins (Fortran, C/C++, Python).

Building blocks: Summary


```
import comin
import numpy as np
```

primary constructor:
request additional ICON variable

```
comin.var_request_add(("my_var", 1), False)
```



callbacks: register function callbacks through Python decorators

```
@comin.register_callback(↵
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def simple_python_constructor():
    global pres, my_var
    print("simple_python_construc
    pres = comin.var_get(
      [comin.EP_ATM_WRITE_OUTPUT_
      ("pres", 1))
    my_var = comin.var_get(
      [comin.EP_ATM_WRITE_OUTPUT_
      ("my_var", 1))
```

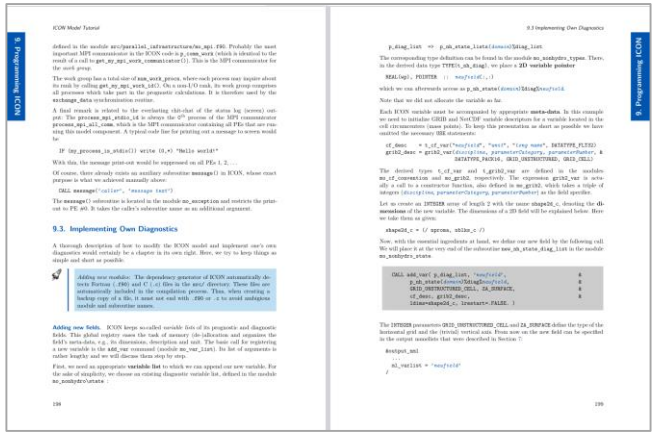
secondary constructor: get variable ha

Compare this to the “heavy-weight” addition of new variables to ICON.

… lots of Fortran CALLs and loops

ComIn plugins are lightweight.

ICON Tutorial 2024 Section 9.4:
Programming ICON / Implementing diagnostics



Fortran and C/C++ API

The previous slides focused on Python. But: ComIn also contains a Fortran and C/C++-API.

Fortran API	C/C++ API	Python API
comin_setup_get_verbosity_level	int comin_setup_get_verbosity_level()	comin.setup_get_verbosity_level
comin_current_get_ep	int comin_current_get_ep()	
comin_current_get_domain_id	int comin_current_get_domain_id()	comin.current_get_domain_id
comin_current_get_datetime	void comin_current_get_datetime(char const**,int*,int*)	comin.comin_current_get_datetime
comin_current_get_plugin_info	int comin_current_get_plugin_id()	comin.current_get_plugin_info
	void comin_current_get_plugin_name(char const **, int*, int*)	
	void comin_current_get_plugin_options(char const **,int*,int*)	
	void comin_current_get_plugin_comm(char const **,int*,int*)	
comin_parallel_get_plugin_mpi_comm	int comin_parallel_get_plugin_mpi_comm()	comin.parallel_get_plugin_mpi_comm
comin_parallel_get_host_mpi_comm	int comin_parallel_get_host_mpi_comm()	comin.parallel_get_host_mpi_comm
comin_parallel_get_host_mpi_rank	int comin_parallel_get_host_mpi_rank()	comin.parallel_get_host_mpi_rank
comin_plugin_finish	void comin_plugin_finish(const char*,const char*)	comin.finish
`n_var_request_add	void comin_var_request_add(struct t_comin_var_descriptor,_Bool,int*)	comin.var_request_add
get	void* comin_var_get(int,int*,struct t_comin_var_descriptor,int)	comin.var_get

Source:

ComIn technical design document

https://icon-comin.gitlab-pages.dkrz.de/comin

MPI communicator concept

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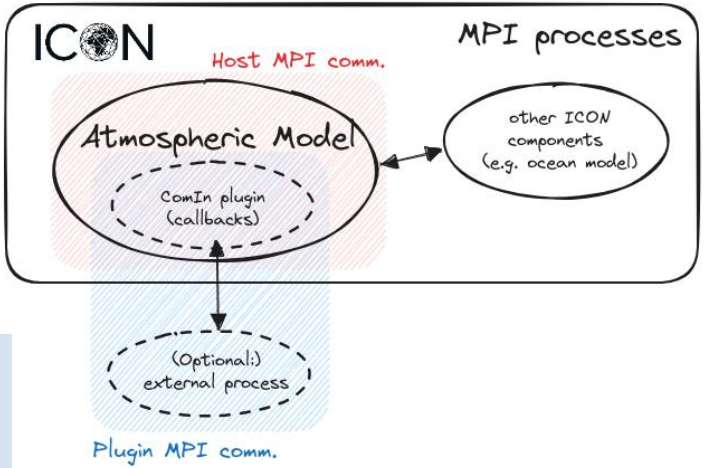
Only process-local partitions can be accessed directly – but MPI exchanges are possible.

Plugins may handle their own parallel communication with the help of a host communicator.



(this translates into mpi4py communicator)

```
comm = MPI.Comm.f2py(comin.parallel_get_host_mpi_comm())
rank = comm.Get_rank()
```

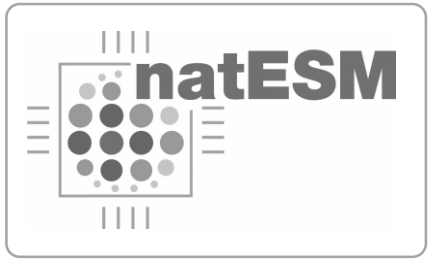
In addition, a plugin communicator (optional) can be created:
Useful for exchanging data with other running processes.

Limitations / Discussion

- ICON calls ComIn, not vice versa!
  - ~ plugins do not influence ICON's restart behavior
  - ~ processes in the host model are not switched off, but can only be deactivated using ICON namelist switches
- Granularity: above block loop level, only global variables are exposed
- access to the process-local MPI partition only (but MPI exchanges possible)
- no asynchronicity between ICON and the 3rd party modules

ComIn is currently under construction. Feedback welcome!

Applications



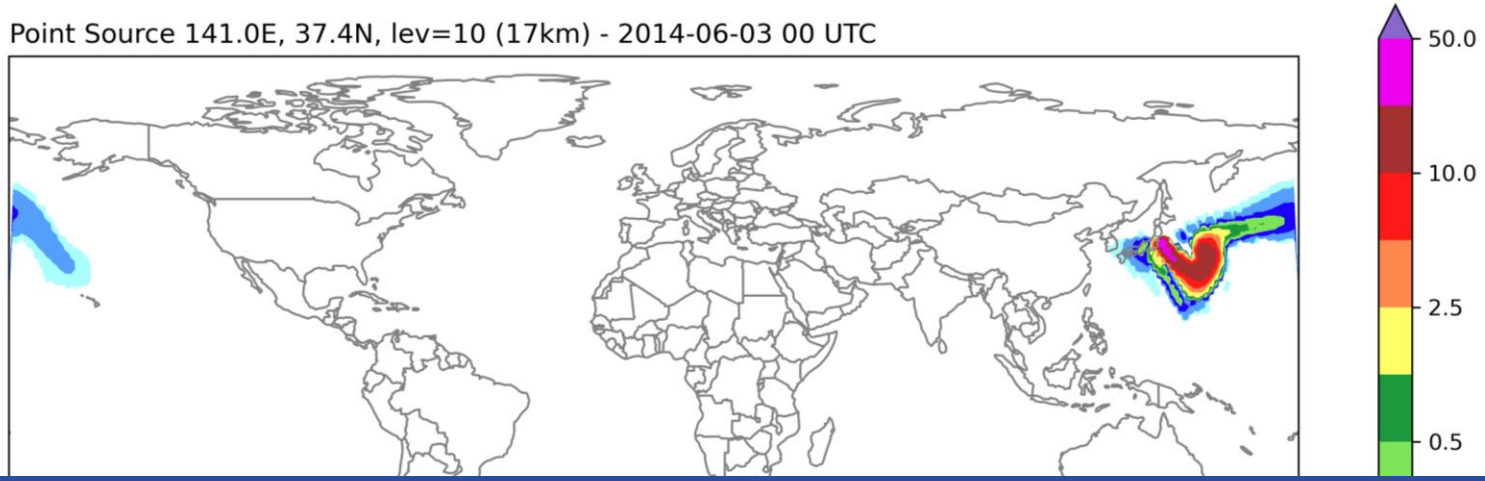
Example plugins

ComIn comes bundled together with several example plugins.

Script name	Language	Description
`simple_fortran`	Fortran	Simple ComIn plugin written in the *Fortran* programming language.
`calc_water_column`	Fortran	Simple diagnostic application, calculating the liquid water path, the ice water path, and the total water column.
`yaxt_fortran`	Fortran	Example plugin to demonstrate the usage of the YAXT communication library.
`simple_c`	C/C++	Simple ComIn plugin written in the *C* programming language.
`yac_input`	C/C++	Plugin written in C which encapsulates a YAC coupling inside a ComIn plugin.
`yaxt_c`	C/C++	Plugin written in C to demonstrate using the YAXT communication library.
`simple_python_plugin.py`	Python	Simple ComIn plugin written in Python, using the ComIn Python adapter.
`point_source.py`	Python	Test plugin requesting a tracer that participates in ICON's turbulence and convection scheme.

Btw.: See the practical exercises for an example how to use matplotlib directly within ICON.

Point source example



ComIn example:

```
python_adapter/
examples/
    point_source.py
```

- request a tracer that participates in ICON's turbulence scheme
- add point source emissions to this tracer
- update the tracer with tendencies received from ICON's turbulence scheme
- exploit Python's vast library of useful modules (here: `scipy.spatial.KDTree`)

Catalyst in situ visualization

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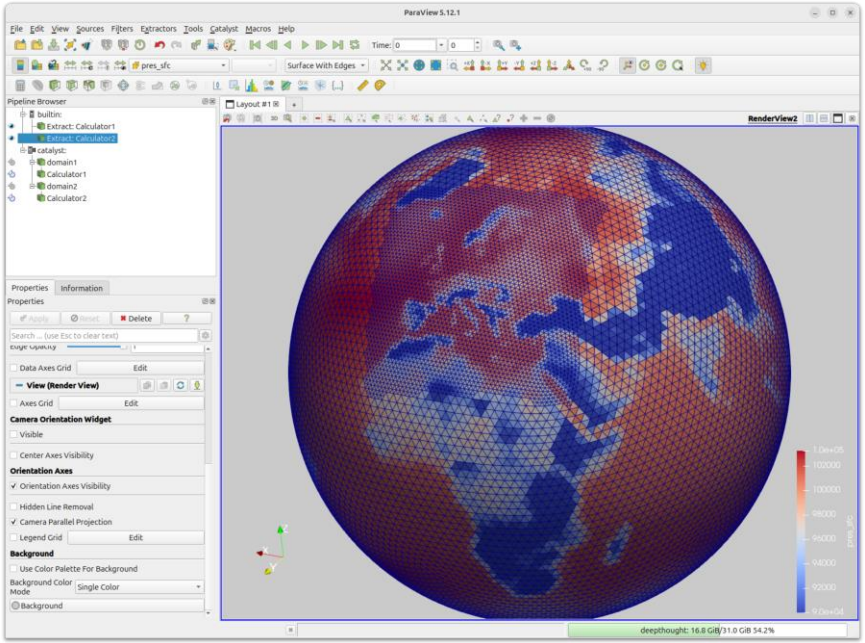
ParaView

Paraview [1] is an open-source data analysis and visualization application.

Simulation data can be streamed into Paraview using the Catalyst API specification.

- application example: Implement the Catalyst streaming for ICON as a ComIn plugin.



Source: N. Dreier (DKRZ)

[1] https://gitlab.kitware.com/paraview

Prometheus/Grafana example

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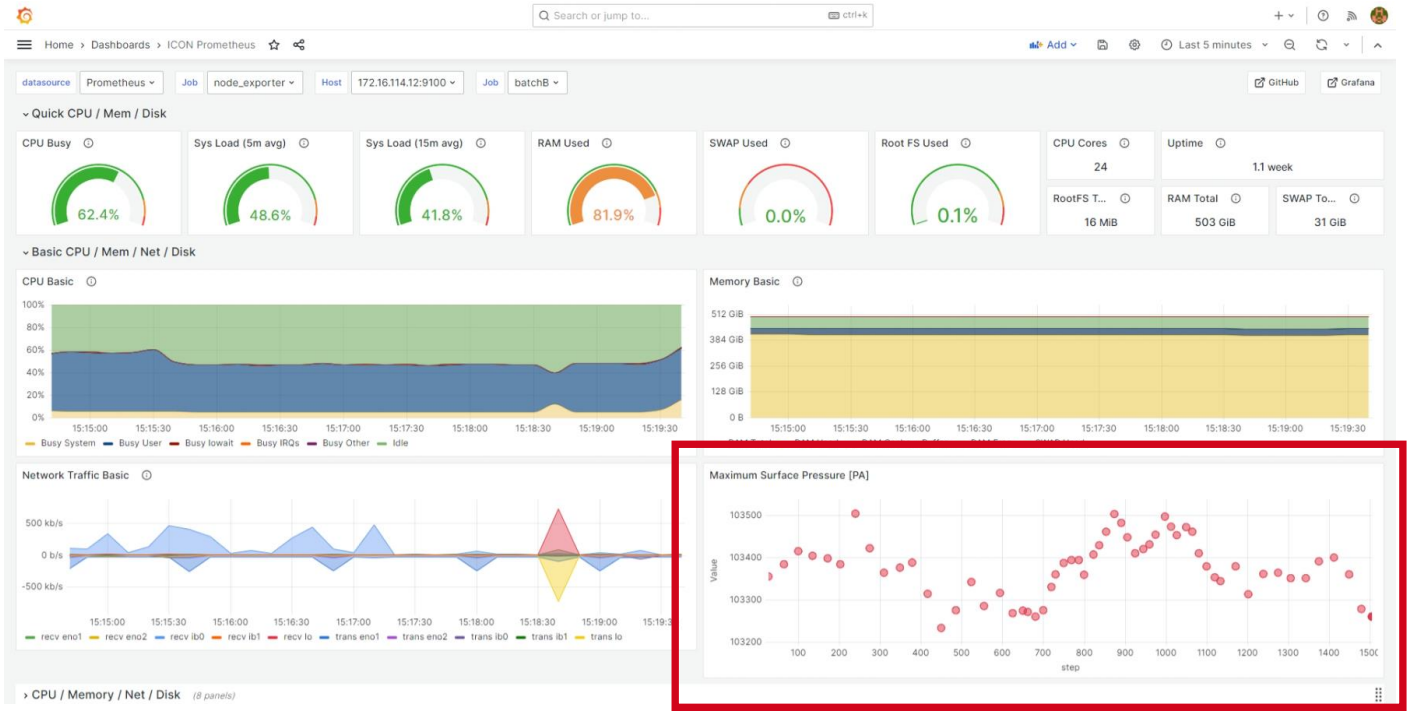
Flexible monitoring dashboard offered by Grafana:



Grafana

Proof-of-concept: connect Grafana to ICON with a ComIn exporter plugin

Ex.: DWD NEC platform displaying ICON's maximum surface pressure

Source:
C. Eser (DWD-TI), FP

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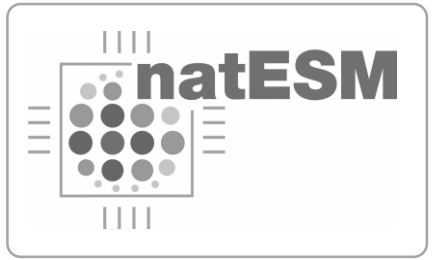
Wrap-up



Roadmap for ComIn v0.2.0

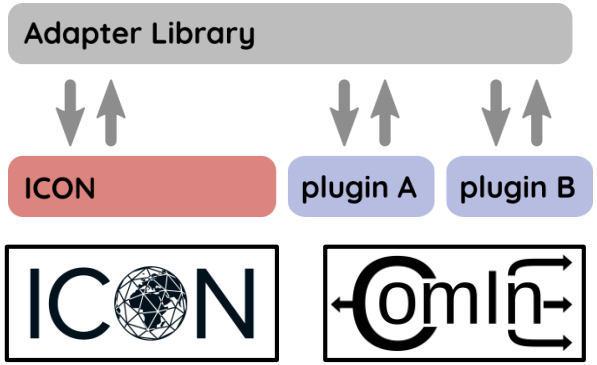
Features that will become available in ComIn 0.2.0
~ August 2024:

- development tool `comin_replay`
  test ComIn plugins with previously recorded data sets
- GPU host-device transfer
- combining ComIn with YAC [1]
  ComIn is an interface, not a translation layer
- generalizations: additional meta-data; edge-based and vertex-based fields, ...

[1] https://doc.redmine.dkrz.de/YAC/html

Contact

- GitLab-Project: https://gitlab.dkrz.de/icon-comin/comin
  - code (including examples and tests)
  - raise an issue
  - contribute (open a merge request)
- Extensive online documentation:
  - https://icon-comin.gitlab-pages.dkrz.de/comin/
  - see also the ICON Tutorial 2024 [1], ComIn: Section 9.5
  - GMD publication (submitted)
- reach out to us: comin@icon-model.org



[1] https://www.dwd.de/EN/ourservices/nwp_icon_tutorial/pdf_volume/icon_tutorial2024_en.html

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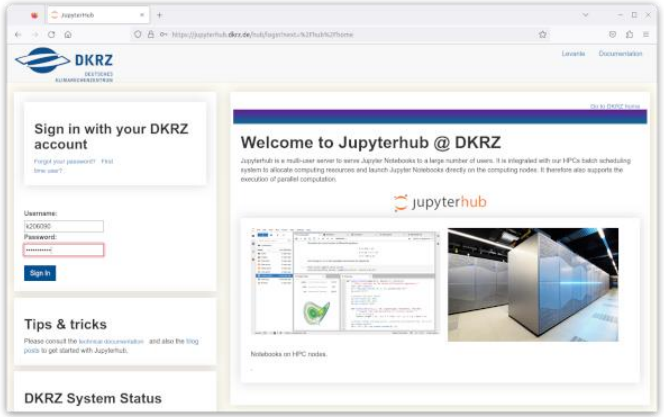
Practical exercises

The exercises are organized as Jupyter notebooks.

- Web site https://jupyterhub.dkrz.de:
  Enter your username and the corresponding password on the start page of the JupyterLab portal.



- In your home directory: Extract course material from with the following command:

```
cd $HOME
tar xfz /pool/data/ICON/ICON_training/comin_exercises.tar.gz
```

- We will be working in the directory
  `$HOME/comin-training-exercises`