

6th Workshop on Coupling Technologies for Earth System Models Q&A document

This document, editable by any participants, is to help moderate questions and support discussions during the CW2023.

During presentations, please write down your questions and comments (with your name, and then initials) in this document, below the dedicated talk. This process allows us to keep track of questions, avoid their repetition and foster discussion.

Session: Coupling Frameworks I

OASIS3-MCT_5.0, the latest version of the OASIS coupler- *Sophie Valcke*

Name: type your question/comment

Olivier: you give conservation figures of about 10^{-4} . I'm a bit puzzled, as we are closer to 10^{-6} with XIOS and IPSL grids.

Sophie: We should check the details of the calculation together. This might have to do with the coastline, which is not perfectly matching in our case?

[Carlos Renato Souza](#): What's your feeling about GPUs in couplers? How are the tests going so far?

Sophie: This should be the subject for a whole session at the next CW! The weight calculation and the remapping per se could be ported on GPUs but this is not planned for OASIS3-MCT; this will be addressed in XIOS. I am not sure if the whole coupler should run on GPUs as some people say that there will always be a mix of CPUs and GPUs on a node and the coupler could remain on the CPUs (as it's workload is relatively small).

Tom Clune: Were the ESMF results with the MOAB grid generation layer?

Robert Oehmke: Nope, the results were just with the legacy version of ESMF mesh.

Uwe Fladrich: I would be interested in the framework to compute regridding weights offline with SCRIP, XIOS, ... Is there any documentation for this, any link? I did not find it in the User Guide or source code.

Olivier Marti : @Uwe : we develop a bit of Fortran, bash and python to generates our weights offline with XIOS:
<https://forge.ipsl.jussieu.fr/igcmg/browser/TOOLS/MOSAIX>

MoritzHanke:

https://cerfacs.fr/wp-content/uploads/2021/11/Globc_TR_Valcke_TR_CMGC_21_145_regridding_analyses_final.pdf

Sophie: Section 6.3.3. of the User Guide, and `regrid_environment_documentation.pdf` in `/examples/regrid_environment`

UF: Thanks for the responses and for the links! However, I am a bit skeptical to see this as a “unified framework” to compute weights online. It seems very specific to running the benchmark test cases, not for the general use for modelers. Maybe a discussion to be continued over a coffee...

Sophie: Yes, you are completely right. I think a tool like the one you develop would be more relevant. It is on my to-do list of things to include in OASIS3-MCT!

Land-atmosphere coupling with ICON and CLM5.0 in TSMP using OASIS3-MCT– *Stefan Poll*

Moritz Hanke: conservative weights are computed by CDO using YAC-code (SCRIP was replaced quite some time ago (SV: ah good that’s what I thought!))...to my knowledge this is the first case of YAC and OASIS being used in the same setup 😊

Stefan: Thanks for the remark.

Olivier Marti ICON time step=10s is for dynamics. Time step for physics, radiation ?

Stefan: Actually the time step mentioned is the one for fast physics. The time step for dynamics is $\frac{1}{3}$ of the model time step (=2s). Slow physics (convection, radiation, subgrid-scale orography drag and gravity wave drag) can be set additionally by the Namelist of the model. In the real case simulation the radiation scheme call is in sync with the coupling frequency.

Joshua Brook-Lawson:

1. Is the output sim data of COSMO directly compatible with the PALM INIFOR preprocessor?

Stefan: I am not so familiar with PALM INIFOR, but to my knowledge it is. Perhaps it would be a good idea to contact PALM people for this question to be on the safe side.

2. Do you have online documentation for setting up a COSMO simulation?

Stefan: Do you want to set up ICON or COSMO simulations? The ICON tutorial is an excellent source for setting up ICON simulation:

https://doi.org/10.5676/dwd_pub/nwv/icon_tutorial2020

Mariana Vertenstein: What type of configuration were you using for CLM (.e. BGC, crop, etc)?

Stefan: Within the TSMP framework CLM is supported in all configuration types. The idealized simulations shown are without crop and no BGC. The real case is running with BGC and with crop function types.

Robert Jacob: Does convergence conclusion (ts < 300s) change if you look at a different variable like soil moisture?

Stefan: Thank you for the question. Indeed the convergence conclusion can be different with the focus on different variables. In the shown case the convergence conclusion does not change by looking at soil moisture in the uppermost soil level.

Tomoko Nitta: Can you explain why the three models are not run concurrently on the page 11?

Stefan: This is done to eliminate the time lag between the atmosphere/subsurface part and the land surface component.

MCT and MOAB in E3SM– Robert Jacob

Jim Edwards - Why did you need another stride variable for the atmosphere? - The CIME PSTRID variable does what you describe.

Rob: seq_comm didn't use PSTRID to build a communicator that gave tasks **exclusively** to the strided component. We could have changed it so that it did but then you couldn't do the "normal" stride. So we introduced exclusive stride. The PR is:

<https://github.com/E3SM-Project/E3SM/pull/4859>

Sophie: You said that support of apps not sharing the same processors was needed for MOAB. Which applications?

Vijay Mahadevan: We have nuclear engineering applications with MOAB that have components that strongly scale well. So our assumption was to run the coupler on all the processes as well for those applications. However, now, MOAB supports both overlapping and nonoverlapping PE decompositions seamlessly.

Rob: Climate, especially the case where you run the ocean on its own processors. That kind of layout never happened in the nuclear apps MOAB started with.

Mariana Vertenstein: When will E3SM start using the new MOAB capabilities by default and move away from mct/cpl7?

Rob: We'd like it in v3.0 but probably won't be ready if v3.0 is released in June this year. That release depends on fixing the aerosol problems so might slip. We will probably do a 3.x release with MOAB as the default since v4 is so far away.

Rob (later): v3.0 is going to be November 2023 so MOAB will be ready for that.

Mariana Vertenstein: Does MOAB permit you to do dynamic masking in the remapping? And what are the mapping types that MOAB supports? By dynamic masking I mean sending a multiple level field to the coupler and having different levels have different masks (think of bathymetry from the ocean that would be sent to the coupler as an example). Maybe dynamic masking is not the right term.

Vijay Mahadevan: What do you mean by dynamic masking? MOAB supports FV-FV, SE-FV, FV-SE high-order maps for arbitrary topology and decompositions.

Rob: I'd have to know more about how you're doing it to say. The ocean surface mesh in MPAS actually has no points where there's land. Its a mesh with "holes". A lower-level mesh would have different size and location of holes so a new intersection and mapping weights could be formed.. That's one way. If you're talking about just throwing away mapping weights at the points that are now holes, that could be done but introduces error.

Vijay Mahadevan: Another way to take care of such a multilevel mesh is to may be use a union mesh to compute intersection once and perform weight generation with specific masked mesh. Note that typically intersection computation is bulk of the work in weight computation for maps. If you have a dynamically moving/changing meshes, then we can easily propagate the changes to the coupler from component and redo intersection/mapping. Doing anything incremental will not preserve accuracy.

Mariana Vertenstein: What motivated E3SM to implement MOAB rather than just using ESMF? It seems that the capabilities are already there in ESMF - are there capabilities that MOAB has that ESMF does not?

Vijay Mahadevan: Rob may have a more detailed answer for this. But our scalability studies in the past have shown better performance for intersection computation and map generation for MOAB in comparison to ESMF. And ability to perform high-order SE-FV/FV-SE was important originally when we were discussing a tri-grid (ATM-LND-OCN) configuration for E3SM.

Rob Jacob: The high-order SE-FV/FV-SE was a big motivator since ESMF can not do that. That motivation went away when the atmosphere introduced the "phys grid" making the coupling FV-FV but by then we were committed. It seemed faster to finish (the other motivations were still there) then to start over.

Kristian Mogensen: Any thoughts on portable GPU programming (OpenMP5?) since you have multi different GPU's on different DOE machines?

Vijay Mahadevan: There are many different choices for portable programming models. OpenMP5 is one choice, but it requires strong compiler

support/implementation on all computing systems and architectures. We are making the choice to use Kokkos as a portability layer so that the interfaces and implementation on higher level coupler remains the same, while Kokkos handles all the gruntwork related to data layouts and kernel launches on CPU/GPU etc. Really no one approach to rule them all IMO.

Rob Jacob: yes we did try OpenMP5 (gpu-offload) in some of the main components but found the Fortran support was not consistent from compiler to compiler

Moritz Hanke: Are there reasons for executing parts of the coupler on the GPU?

Iulian Grindeanu: we are not trying that yet, and it may not make sense ever; we would need much higher resolutions to see any advantages on using GPU for the relatively small-size calculations on the coupler (intersection + map generations is one time op, projection spMV is already distributed with MPI, etc)

Vijay Mahadevan: There may be advantages in performing SpMV on the GPU but the operation is still memory-bandwidth limited. So unless bulk of the physics is actually running on the GPU itself, the data copy between CPU and GPU may start dominating. And doing MPI communication from GPU may not be too stable and hence the copy above is mostly unavoidable.

Moritz Hanke: What percentage of the overall time is spent in the coupling infrastructure?

Iulian Grindeanu: we will do more studies; right now, initialization is expensive in cpl7/mct (create all those GSMaps, reading the maps, computing the routers) , but runtime is pretty efficient. The good news is that MOAB coupler does not add much cost to either phases, which means init phase will be much more efficient when we will remove mct/cpl7 scaffolding; in terms of raw percentages, it is relatively small (CPL is few percents of total cpu time for a relative long simulation) for example, can you see these details (MoHa: yes, thanks!)?

<https://pace.ornl.gov/exp-details/127706>

Latest developments in ESMF– *Daniel Rosen*

Rob: what would happen if you tried to couple 2 NUOPC components that had no fields in common (needs or provides)?

Gerhard: If you put a connector between them, it would notice that there are no fields connected and turn into a no-op.

Dan: Note - By default the NUOPC-layer will fail if a component advertises an import field that does not find a connection (the connection can be satisfied by any of the connections). You can check connections during the realize phase of initialization and make adjustments.

Rob: Does ESMx have to make assumptions about how code in the NUOPC components is laid out in directories to build them together?

Gerhard: It does not assume any special layout if you are providing the CMake config file for the model component in the build yaml file.

Rob: ok that makes sense.

Dan: We're adding features to the ESMX build system to bypass the need for a CMake config file.

Rob: just a note, the "Xgrid" is also the "intersection mesh."

Carsten Lemmen: What about CMake for core ESMF build?

Gerhard: It is a funding question and up to the CRB to prioritize with the resources available. We do have Windows ports also in the GNU based build system.

Andrea: about the flexible hybrid parallel layout, are you in touch with the [Quo-vadis](#) project (Edgar Leon at LANL and Samuel Gutierrez at LLNL)? They are carrying it to a higher level of abstraction. I quote: *A next-generation, machine-independent coordination layer to arbitrate access among multiple runtime components and map tasks efficiently to heterogeneous architectures.*

Gerhard: No, we have not looked into that. Thank you for the link, will have to take a look.

Sophie: Are the problems we noticed during the benchmarking still on your "to-do" list? 😊

Robert Oehmke: Yes, although now that I've seen them again, they've risen closer to the top. :-) (Sorry, it's been a busy couple of years, so I haven't circled back to them yet, but they are definitely on my mind.)

Sophie: great, thanks. No pressure because I think they are not a problem for any specific group right now.

Robert Oehmke: Thanks. That's good to know, but I will try to take care of them as soon as I can. :-)

Carsten Lemmen: I am really enthusiastic about ESMX, what is the status about its documentation (reference guide and user guide)

Gerhard: Currently documentation is README.md based. Primary under ESMX level on GitHub ESMF repo: <https://github.com/esmf-org/esmf/tree/develop/src/addon/ESMX>

This covers the ESMX prototype that came out with 8.4.0. Notice that the layer is under active development. Long term, once ESMX is considered more mature, we plan to provide a more formal ESMX Ref Doc.

MAPL3: A hierarchical framework based on ESMF– Tom Clune

Sophie V: Regarding regridding tangent vectors, each component u or v (spherical or local coordinate system) should not be regridded independently. But the vector should be projected in a cartesian space and the resulting 3 components should then be regridded and then projected to the target grid in the spherical or local coordinate system. Do you support that?

[Robert Oehmke](#): Just a note, we're working on bringing the vector regridding functionality that you describe into ESMF regridding, so it's good to hear that you use this too!

Tom Clune: How will users indicate to NUOPC that a quantity is a vector (pair of fields) rather than just 2 scalars? I.e., are you planning to have default connectors that deal with this or just additional ESMF level calls for explicit regrids?

Sophie: We are not supporting vector regridding in OASIS3-MCT (but we did in OASIS3); we just warn the user about how to do this and we suppose that the fields sent are one of the 3 components in the cartesian space. We backed up on this as associating a pair of fields in the coupler brought a lot of complexity and we think the transformation from local to cartesian coordinate system was quite easy to do in the code (as it is done in NEMO for example).

Carsten Lemmen: In your comparison table, you mentioned that MAPL is *not* a community infrastructure (if I saw correctly). Is there a reason for that (seems a bit odd in comparison to every other system presented here)? What about the user base?

Tom Clune: As I briefly explained at the end of the talk, we are not funded to provide support to external communities. ESMF/NUOPC is the community framework, and NASA is very explicit that support \$\$ go to the ESMF core team. We do however support scientific collaborators such as Harvard GEOS-Chem and NOAA UFS. We are also on GitHub and don't ignore issues raised there, but in practice those are all by collaborators.

Carsten: thanks Tom, I guess we have similar issues that there is often not funding for sustainable community support . A great problem with project funding for infrastructure development.

Tom Clune: I should say though, that my group is itself adequately funded, and best of all, do not need to even write proposals to sustain that funding. We are carved a slice of the GEOS budget to support it with smaller supplements from research grants by individual scientists.

Infrastructure for next generation community models using ESMF/NUOPC – *Mariana Verstenstein*

Rob Jacob: Which country/institution is COSIMA?

Mariana: Australia. They requested a CMEPS presentation and want to use it.

Rob Jacob: Would like more info on what “dynamic masking” is (also mentioned above in my talk).

Iulian: is it about using different masks for ocean depending on level of ocean ? deeper level might mean a different mask at that level ? compared to surface level ? would that mean that the coupling happens not only on the surface / bottom atm / top of ocean ? Or dynamic means changing coastline at runtime ?

Gerhard: The ESMF feature is “dynamic masking”. It can be used for temporal changing masks, or as Mariana is describing for mask info changing by level.

Carsten: we're using (=trying it ...) it in NOAA/NOS's CoastalApp for compound flooding, i.e. National Water Model (runoff, routing) shifting coastline and interface to ocean model SCHISM

Tom Clune: GEOS uses it for output when some model levels go underground.

Rob: these mask examples make sense. Still not sure what is actually being done with the mask.

Sophie: Does the use of NUOPC (or MCT) caps prevent in-line (within the time step) coupling exchanges and therefore constraint the coupling algorithms that you can implement?

Gerhard: More frequent coupling is often done by introducing multiple run phases.

Rob: The cpl7/MCT cap doesn't know/care what happens inside the model under the cap.

Sophie: Thanks, Mariana and I will have a chat about this tomorrow!

Vijay Mahadevan: Is the time interpolation used to provide flexibility in when the rendezvous exchange happens? Or is it done to recover a higher order coupled field even if the underlying component uses a low order temporal integration scheme?

Mariana: @Vijay - I don't understand your question. Are you referring to CDEPS? There is no time interpolation in CMEPS. You need time interpolation in CDEPS because the forcing data will generally have time stamps that are not at the model time stamp - so you need to interpolate in time as well as space.

Vijay Mahadevan: Ah, understood. I was under the impression that this was a general capability used in CMEPS as well.

Towards an Exchange Grid Implementation within the UFS– *Ufuk* ***Turuncoglu***

Iulian: Obs: ‘exchange grid’ is intersection grid in MOAB

Gerhard: It would be interesting to compare ESMF XGrid with MOAB intersection grid, e.g. do they both allow multiple grids on both sides?

Iulian: not sure I understand this question. Intersection is carried between 2 different grids, 2 different models, one source, one target; multiple grids on both sides would mean multiple grids on source, and/or multiple grids on target? For each coupling between a target grid and a source grid, we have an intersection grid. So total number of intersection grids would be number of target grids times number of source grids. Or would be the number of desired combinations source-target. Again, not sure I understand the question

Sophie V: Can you summarize the climate impact (or no impact) of using the exchange grid?

Mariana (transcribed by Rob):: Didn't see any impact when using standard resolution climate runs. Could have an impact on refined grids.

Ufuk: Hurricane forecasts might show an impact. It has not been tested yet.

Carsten: we will likely need to test this in CoastalApp, I guess your expertise is then sought.

Ufuk: Sure. I have just started to work on a CoastalApp project that aims to sync it with UFS WM and other staff. We could talk about more if you want.

Session: Coupled Systems / Science of Coupling

MIROC-ILS coupling: Coupling multiple land component models to an atmosphere and ocean model with Jcup— *Tomoko Nitta*

Iva K: How are data passed between ILS and the land models it couples? Did the land models also need to be adapted to work with ILS interface?

Tomoko Nitta: Thank you for your questions. All land component models call subroutines of the interface (ILS coupling interface) over the Jcup library.

Sophie V: Why did you develop SPRING instead of using one existing library? Does SPRING calculate the weights on-line in JCUP or do you use SPRING to pre calculate the weights?

Tomoko Nitta: We needed a tool to allocate the basin-shaped land grid while following the land-sea mask of our ocean model. But unfortunately, we did not find such a tool at the beginning. That's where we began the development of SPRING. And then, it evolved into the regridding tool. We use SPRING to pre calculate the weights.

Sophie V: In MIROC-ILS, all the components are separate executables?

Tomoko Nitta: Yes, they are.

Kristian Mogensen: How big is the science impact of running the land model at higher resolution than the atmosphere model? Does each land grid point have only type or is there a subgrid parameterization?

Tomoko Nitta: We are working on evaluating the simulation results. We expect that higher-resolution simulations will improve the reproducibility because hydrology is greatly affected by topography, and higher resolution allows us to consider more complex surface conditions (e.g. land use distribution, LAI, soil distribution, etc.). Each land grid point has multiple land surface type with subgrid parameterizations (e.g. snow cover fraction), but we think it is not sufficient.

Jan Streffing: Do you attempt to make use in a stochastic manner of the information that is available on the land surface grid, which would be considered subgrid-scale for the atmosphere?

Tomoko Nitta: Currently, we use the area-weighted average. But it's an interesting idea; I will think about it. Thank you!

The UKC3 regional coupled model– *Juan Sanchez*

Kristian Mogensen: Do you use the NEMO wetting and drying due to tides and does that change the LSM in NEMO when coupling?

Ségolène Berthou: As Juan was saying, at the moment the LSM is fixed, and we're testing extending the land mask into the ocean and ocean mask into the land and passing the sea surface height at the coast from ocean to land. Also using NEMO "geothermal heating" capability to actually pass the land flux to the ocean near the coast (where the land is heated by the atmosphere under a thin layer of water). This is still being tested, thanks Sophie for highlighting the new time-evolving land-sea mask capability.

Kristian Mogensen: Is the sea-ice model active in your system?

Ségolène Berthou: No (as Juan said), but the Bureau of Meteorology in Australia is planning to create a regional domain over the Antarctic, so we'll add it at some point.

Kristian Mogensen: Is this system currently used or planned to be used for short-range NWP?

Juan M Castillo: This is a research system, but parts of it are being used in operational NWP models at the Met Office, for example the ocean/wave coupled configuration. They will be incrementally added to the rest of the operational models, not only the UK model but also there are plans to implement it in other operational domains such as India and Singapore.

Ségolène Berthou: Planned to be fully coupled operational around 2028. - but at the moment the operational atmosphere, high resolution atmosphere degrades the wave and ocean forecasts (too strong winds, not enough radiation in summer). We're hopeful that our most recent Regional Atmosphere version will improve both.

Kristian Mogensen: Juan+Ségolène: Thanks so much for your detailed answers. Would you be interested in having a more detailed online discussion on these aspects? At ECMWF we will touch upon similar problems/issues when we run the very high resolution global systems and exchange of ideas could be interesting (at least for me ;-)).

Ségolène & Juan: Yes Kristian, it'd be great to have a chat, please can you email us segolene.berthou@metoffice.gov.uk, juan.m.castillo@metoffice.gov.uk ? Thanks for your interest.

Kristian: I will contact you. Thanks for the talk. Talk to you later.

Ha Hagemann: which NEMO version are you using? Do you transfer turbulent fluxes from your atmospheric model to NEMO?

Juan M Castillo: we are using NEMO 4.0.4, but this year we will be moving to NEMO 4.2 and will add extra flux exchanges and wave science that is now available. Biogeochemistry coupling is only supported in NEMO 3.6 at the moment.

Ségolène Berthou: And sorry we couldn't make it in person, it's the week of the science review at the Met Office so it's very busy...

Prognostic Schemes of Skin Sea Surface Temperature for ocean-atmosphere— *Vincenzo de Toma*

Ha Hagemann: the Hydrological Discharge (HD) model belongs to Helmholtz-Zentrum Hereon. It can run as a stand-alone model as well as can be coupled to other models via the OASIS3-MCT coupler or the YAC coupler.

Vincenzo de Toma: Sorry for that, I will remember it better next time!

Aurore Voldoire: Have you checked in NEMO at which depth you can see an effect of the diurnal cycle?

Vincenzo de Toma: definitely in the first layer.

Vincenzo de Toma (Corrigendum): Actually one of the inputs of the warm layer routine within NEMO is the warm layer reference depth, which by default is fixed to 3.0 m. I have not checked in my control run where is the depth at which the diurnal cycle can be neglected, but I will take into account this comment in developing a future simulation, Thanks!!!

Jan Streffing: Does NEMO support a control simulation with very high vertical resolution in the top ~20m? I have seen such simulations with ICON-O. Might be of interest to chat with folks from the TRR181 project that do research on impact of diurnal warm layers:
<https://www.trr-energytransfers.de/research/area-1/reports/14>

An Assessment of coupling of CFS model with SSiB Land surface model on regional Climate— *Nagaraju Chiluktoi*

Jan Streffing: What ensemble size was used for determining the impact on 850hPa wind patterns?

Nagaraju: each experiment has four ensemble member mean

RegCM-OASIS-Symphonie air-sea coupling in Southeast Asia: development, parameterization and strategy— *Quentin Desmet*

Øyvind Seland: How do you include the boundary conditions?

Kristian Mogensen: Maybe I missed it, but what kind of boundary relaxation do you use for both ocean/atmosphere (same question as Oyvind I guess)?

Quentin Desmet: I'm using exponential relaxation with ERA5 in the atmosphere. For the ocean, it's more difficult to say for me right now. I use COPERNICUS with a relaxation profile depending on the forcing current but I need to look for the type of profile exactly.

Kristian Mogensen: Just a warning. Even reanalyses are not perfect.

Quentin Desmet: Yes, I got it. Do you target the boundary condition forcings when you say that or the comparison for validation (or both)? When it comes to forcing, I think reanalysis is better than other options like global model outputs, would you agree?

Kristian Mogensen: Reanalysis is the best we have, but it is worth doing a literature search to see if others have complained about ERA5 in the South China Sea area. I know that the precipitation is not good for the Maritime continent.

Ségolène Berthou: Very nice work, Quentin, we actually have also developed a regional coupled model at 4.5km over a similar domain to yours, it'd be nice to catch-up at some point. segolene.berthou@metoffice.gov.uk

Quentin Desmet: Thank you Ségolène, I'll contact you soon then.

Dan Copsey: An important source of clouds is boundary layer turbulence. I noticed that some of your biases are around the islands where boundary layer turbulence is important. I don't know what boundary layer scheme you use but maybe tuning/improving that might be something to try. dan.copsey@metoffice.gov.uk

Quentin Desmet: I thank you for your comment. I also noticed these patterns around lands. They seem to be influenced both by the moisture scheme and the PBL scheme. Concerning the PBL schemes, I have the choice between the PBL from Holtslag *et al.* (1990); the UW PBL from Bretherton & McCaa (2004) – which I am using; Mellor & Yamada (1982) (with the note Janjic, 2002); and the one from 2011 NCEP GFS. I will make sure I explore all the options as you point out the importance of this aspect.

Modeling systems in modeling systems in modeling systems - FABM in SCHISM in CoastalApp– *Carsten Lemmen*

Marc Stringer: Thanks for answer. I think the main problem with FABM was that MEDUSA is an intermediate complex ocean biogeochemistry and it assumes fast descending detritus reaches the bottom of the ocean in one timestep, and FABM didn't like transporting detritus all the way to the bottom in one timestep. It also required a significant re-write of MEDUSA, and by the time this was done the trunk version of MEDUSA had evolved a lot. And I think the overhead was something like 5/10% for MEDUSA, and no one seemed be available to maintain this software.

Carsten: FABM itself is maintained by Jorn Bruggeman. There is good support for Q&A in the community. The maintenance of the individual models (e.g. Medusa)

happens on your side. You can subcontract Jorn's enterprise to do development for you, if you'd have the money. We have also had trunk divergence issues. I think the way to go is to refactor your model with FABM structure in mind (but not the interface implemented), changing the internal structure only first. Then in a second step at the FABM API calls.

Carsten: As for the fast sinking, we've had problems with that as well with detritus falling "through" multiple ocean vertical levels, predominantly at river/ocean interfaces. We dealt with this by horizontally distributing the detritus river input along the entire width of the estuary rather than seeing the river as a point source. As FABM is in principle only looking at one cell at a time, you have to make sure that the CFL is observed for sinking.

Marc Stringer: thanks Carsten. A major hurdle is the chief architect of MEDUSA, Andrew Yool, really doesn't want it - so I doubt it will be used with MEDUSA. He can see the overheads and not much gain.

Carsten: It's also about resources, I guess. Yet one of the strongest advantages of FABM is not yet utilized in science, i.e. the potential to compare different BGC in the identical ocean model. For the ecosystem/ecology/biology community, this capability is important, especially when we want to use those models to inform policy about carbon storage potentials. A project to do that, comparing PISCES, CoSINE, Medusa, ERSEM (to name a few big ones) each running in each of the major ocean models make a great contribution to our field, IMHO, but would consume significant resources and require collaboration. As with all of the coupling systems (FABM, but also ESMF, OASIS) there is an overhead.

Marc: fair point, thanks - but I still don't think Andrew Yool will be convinced.

Carsten: I don't know about MEDUSA, but one of the strongest aspects next to intercomparability and reduction of interfaces is the coupling ability within FABM. So you can have different BGC models (e.g. light, spm, n, p, z, d, alkalinity, filter feeders) all coupled (within the FABM framework) and still having only one interface in your ocean model. So the granularity can be driven to extremes here ...

Tom Clune: Are there particular capabilities of FABM that would not be practical with ESMF? Or is this simply a different framework emerging in a subcommunity?

Carsten: FABM is a box model without space awareness (apart from a concept of surface/bottom), it relies on the so called "host" (the ocean model) to advect/diffuse it's tracers and do (or forward) the I/O. We have in our MOSSCO coupling system an ESMF component of FABM (both for an in-sediment and for a pelagic version), which we use in many of our simulations. But to <https://weather.cod.edu/satrad/nexrad/index.php?parms=LOT-N0Q-0-6-100-usa-rado> this, we had to create additional hooks into our ocean model (at that time GETM) to advect the tracer fields. So yes, it works.

From a legacy point, however, and as many ocean models have rather a FABM interface than a generic "ESMF gives me a field bundle which I have to transport" interface, I guess it's ok to leave it at the current levels of modularity.

Mariana Vertenstein: What is the current status of the NOAA Coastal App in terms of default components - and what are the plans (development and evaluation) to migrate to SCHISM or some of the other components listed.

Carsten: SCHISM (3D) will replace ADCIRC (2D) for operational compound flooding

Sophie: what is the advantage of using NUOPC if your coupled system MOSSCO was already running with ESMF? New components?

Carsten: Several advantages (1) less code to maintain (the SCHISM ESMF interface is 4000 lines of code, the NUOPC is 1000); (2) better integration into existing coupled systems, most of which are nowadays NUOPC not ESMF, so yes, new components. (3) No need to maintain our "link_coupler", "regrid_coupler" (which is now automated in NUOPC). But, I have to say, I still feel I have better knowledge (and feeling of control of what's going on) with ESMF rather than NUOPC.

Dan Rosen: NUOPC is used to couple to/within the CoastalApp, which is part of the Unified Forecast System (UFS) environment. The UFS environment uses NUOPC.

Mariana Vertenstein: The UFS system is also using CMEPS and CDEPS.

Tony Craig: System looks technically flexible with respect to components, is the science robust too or is there a lot of tuning needed as new configurations are run?

Carsten: Which system are you looking at? The old (MOSSCO) system is robust and has been validated with data in different coupled constellations in a variety of papers, all on the North Sea coastal system. The new ocean model SCHISM itself is validated quite successfully, mostly scored against tidal and river gauge data for past hurricanes. The CoastalApp coupled system is (using the new SCHISM-ESMF) in development; we're not yet at the validation stage.

Links for the above discussions:

- FABM <https://github.com/fabm-model/fabm>
- SCHISM <https://github.com/schism-dev/schism>
- SCHISM-ESMF <https://github.com/schism-dev/schism-esmf>
- MOSSCO <https://sourceforge.net/p/mossco/code/ci/master/tree/>
- CoastalApp <https://github.com/noaa-ocs-modeling/CoastalApp>

Maintaining hydrostatic stability when coupling ROMS' ice shelf to an ice sheet model— *Stefan Jendersie*

Ségolène Berthou: Just a comment. Thanks for your presentation, highlighting a complex numerical issue! You may be interested in this article, where they've changed the vertical coordinates of shelf-NEMO to reduce spurious horizontal pressure gradients that you highlighted <https://www.sciencedirect.com/science/article/pii/S1463500321001827> (though I appreciate it's a simpler problem as there's no "topography at the top of the ocean" in this system!

S.jendersie - thank you for pointing this out, I was not aware of it.

Rob Jacob: bash script coupling? Does this mean coupling by files? (answer: yes). Have to reconfigure ROMS each time.

S.Jendersie: not really reconfigure. But essentially the coupler automatically builds a new ROMS bathymetry / ice draft / ice-ocean-land mask / vertical coordinate system at every coupling stage.

Iva Kavcic: Do you couple PISM with ROMS for every ROMS timestep within PISM timestep? Also, do you need to adjust PISM timestep if there are instabilities or is it handled by smoothing?

S.Jendersie: The ocean runs at a baroclinic time steps of 20 min which is near the theoretical limit. We limit PISM time step to one year to do the coupling. It could run at larger time steps but PISM computation demand for one year is negligible compared to what ROMS needs.

Carsten: Thanks for the comment about data and truth :=)

De rien 😊

Vijay Mahadevan: We are working on coupling MPAS and ROMS regionally through a DOE funded project. There may be opportunities for collaboration especially in adding a new coupler for your workflow.

S.Jendersie: Hi Vijay, I would be very keen to have a conversation for sure. Are you here in Toulouse or online?

Vijay Mahadevan: @jendensie I'm online but work with jacob@anl.gov on E3SM coupler. We can have a detailed chat soon. Please feel free to email me at mahadevan@anl.gov.

Time schemes at the ocean-atmosphere interface – *Olivier Marti*

Juan Castillo: Would this be necessary if the boundary conditions are time interpolated ?

Olivier To suppress the problem, one needs to extrapolate in time, not interpolate. And we have check that extrapolation of boundary conditions does not give good results, with large error after sunset and before sunrise. We have tested 1st, 2nd and 3rd order extrapolations.

Valentina Schüller: How does the error develop over the course of the 5-day simulation? Does it start small and get worse later during the simulation or does it stay similar in magnitude?

Olivier To update the models at each time step, we use the tendency computed by the Schwarz scheme. The tendency computed by the legacy scheme is computed for diagnosis, but not used. So there is no accumulation of error over time. We have only one trajectory of the model.

Vijay Mahadevan: More of a comment. There has been prior work done in using multiple Picard type iterations to converge nonlinearities between coupled components. Depending on the nonlinearity, two iterations should yield relatively better stability, and so the result supports the conclusion.

Vijay Mahadevan: If you are working with just two components as in this example, you can try Strang splitting with the Schwarz scheme to yield a second order coupling method. I am curious whether this has been tried previously.

Kristian Mogensen: If all models can run on the full number of tasks/threads then you would be good with sequential atmosphere first coupling since you can use `nproc_atm+nproc_ocn` from your parallel coupling for seq coupling.

Olivier Our ocean and atmosphere does not run on the same number of processors to have the same execution time. I cannot not increase much the number of procs used by each component. In a sequential run, we will be obliged to reduce the number of procs, and increase the time to solution.

Sophie: You could implement atmosphere-first and still run your components concurrently if you agree to have a lag of 2 coupling period. This is [the algorithm implemented by Environnement Canada](#). You get the benefit of the atmosphere-first algorithm and the performances.

Jan Streffing: I think for simulations where time to solution is a problem, one would have to weigh the increased cost, which you would have to save in model resolution or ensemble members. Increased error via parallel coupling, vs increased error from reduced model complexity / ens members / degrees of freedom

Rob Jacob: comment: Some models (CESM, E3SM) can run atmosphere and ocean on the same processors so wouldn't have the wasted processors in an atmosphere-first scheme. (note to self: try this with E3SM)

Olivier : but you increase the time to solution. Might be OK, in particular if you run several experiments in parallel.

Rob: Our 1 degree fully coupled model can do about 40 years/day on an AMD cluster. 20 years/day would still be great.

Stefan Poll: Are your ATM-OCE model coupled with instantaneous values?

Olivier : we average all variables over the coupling time step. For $dt=1h$, that's 2 ocean time steps, 1 sea ice time step, and 4 atmosphere time steps (slow physics). Radiation computation is done every coupling time step.

Session: Performance

High Resolution Coupling with OpenIFS-FESOM2– *Jan Streffing*

Kristian Mogensen: Is it really similar resolution since IFS uses a structured grid and FESOM2 uses an unstructured grid? Are there any special issues to consider for this combination? (Question kind of answered on the stoch. coupling slide).

JS: In general we are closer than we would be with ECHAM6, but indeed there are large spatial variations in resolution ratio within setups. The stochastic coupling is one idea to take that into account.

Rob Jacob: just a comment: E3SM also had to deal with this missing enthalpy because precip on the ocean (MPAS) actually adds mass to the ocean (but heat was not tracked).

Mariana Vertenstein: CESM just had to deal with missing enthalpy as well. It has been partially addressed in the mediator with new corrections applied.

JS: Good to know we are not the only ones ;-)

Stefan Jendersie: Does FESOM have an option to add ice shelves / subglacial melt water discharge? You did mention an ice berg module.

JS: Yes FESOM2 has something called max-mesh, where we can turn certain points wet/dry and generate subglacial meltwater and heat fluxes in the cavities.

Rob Jacob: which machine gave you 8 SYPD on the DECK Setup?

JS: This one was done with ICCP on the aleph system in Busan Korea:
<https://ibsclimate.org/research/facilities/aleph-supercomputer/>

Mariana Vertenstein: What is the vertical extent of the atmosphere (how many vertical levels)? Is there a biogeochemical cycle used in the lnd/ocn - and chemistry in the atm? What about using the exchange grid instead of the stochastic coupling?

JS:

- We use TCo95L91, TCo319L137 & TCo639L137, so 91 or 137 vertical layers
- We have FESOM2 RECOM obgc coupling, but it was not turned on in these runs and coupling to Atmosphere Dyn Veg Carbon cycle is TODO for the next ~2years
- Atm Chem is not yet in the model. We are going to have CAMS for OpenIFS43r3, and eventually move to OpenIFS48r1, which should come with chemistry.
- We have not thought about exchange grid. I assume this means making the FESOM data available inside the OpenIFS model on its original unstructured mesh?

Ha Hagemann: what is Runoff mapper?

JS: It's a very simple "model" that reads two netcdf files, one with drainage basins over land, one with arrival points over the ocean for ~70 basins. No ability to store/release water though.

Moritz Hanke: Could you use the "nearest destination to source"-interpolation method to do this? (SPMAP in YAC: https://dkrz-sw.gitlab-pages.dkrz.de/yac/d3/d41/interp_method_spmmap.html)

JS: We could, but I think having the real destination mapped is a step better than mapping to the nearest ocean point, no?

Vijay Mahadevan: Why use a stochastic remapper? Why not use deterministic field gradient based metrics at runtime to decide high vs low order choices etc from an array of available weights for each DoF?

JS: Interesting idea, I will think about it some more. My first thought is, that storing multiple available weights would be more intrusive in terms of modifying oasis infrastructure.

VM: I think the concern would be the memory overhead of maintaining multiple weights. But certainly for fields that evolve during the simulation considerably, I think such a scheme could be useful.

Carsten Lemmen: I recently heard a lot about FESOM-C a coastal version of FESOM. How much is the development overlapping? And seeing you're going down to 2 km scale, why would you have a separate coastal model at all?

JS: The two code bases are fully split and use different numerical cores. Afaik the down to FESOM-C group is working on tidal channel resolving setups. Indeed we are getting into similar areas though. Every once in a while the idea of implementing a FESOM-FESOM-C coupling/nesting is cropping up. Nothing concrete though.

Carsten: Is there a fundamental reason why your variable ocean resolution does not span more than 1 order of magnitude (often less)? Why not 100 km in tropical gyre and 10 m at Bremerhaven harbour (just for example)?

JS: There are diminishing returns of saving computing resources by coarsening in uninteresting parts. If we put 10m resolution in the North Sea and 100km elsewhere, 99.9% of all grid points are in the North Sea and the time step will be 1s or so. In that case why not spend 10% more resources and have the rest of the ocean at 100m? :)

Coupling at Scale: Experiences from the INCITE project – *Kristian Morgensen*

Rob Jacob: why develop a custom coupling solution for the ECWMF coupled model?

Kristian: Answered I believed.

Rob: Yes.

Iva Kavcic: An offline tool to calculate communication patterns sounds interesting. Is it targeted at your application of weights interpolation? Can it be used for others as well?

Kristian: Discussed at coffee

Iulian Grindeanu: did you try pnetcdf to read in parallel ? with MOAB, we read netcdf files in parallel and re-distribute them with an online partitioner (Zoltan)

Kristian: Haven't tried. Good suggestion

Niki Zadeh: What was your GPU utilization strategy for Summit? Directive base (openmp/openACC) or rewrite in C/Cuda/kokos?

Kristian: we use CUDA for the spectral transform on Summit.

Moritz Hanke: ICON-ESM does not use weight files. Weights are generated online by YAC at startup, which is faster than reading the weights.

Kristian: Noted.

Carsten: I am mildly shocked by the announcement to build more postprocessing/output capabilities into NEMO. Shouldn't this be left to dedicated outputs servers, that could do this much more efficiently, more general and are already existing?

Kristian: The one we used was already there. We used the observation operator code developed by the NEMOVAR team (ECMWF/CERFACS/INRIA/MetOffice) for data assimilation. Sorry if that was not clear.

Stefan Poll: Are you adapting the model parameterizations with the change of horizontal grid spacing?

Kristian: Yes, but only for the deep convection in the atmosphere.

Automatic approach to balance coupled ESMs - Sergi Palomas

Rob Jacob: in your iterative process, how do you modify the processors?

(answer: move processors from fastest to slowest component. Only doing 2-component systems so far.)

Harry Shepherd: What do you consider a “good” coupling cost, for a simulation with (for example) 2 components?

Sergi: That really depends on the applications that you are coupling. But from the performance metrics we got for the whole CMIP6 exercise, people reported between 10-20%. But I believe that a good one should be less than that.

As I said, however, for EC-Earth we are more than happy with 10% due to IFS computing the radiation (having irregular ts lengths) every 4 ts (3h) while NEMO ts are always equal.

Kristian Mogensen: ECMWF is the new ATOS machine?

Sergi: No, the previous one (CCA)

Jan Streffing: How long is each iteration simulation? How much computing time is spent optimizing? Do you have to make repeat tests?

Sergi: This can vary from application to application and also depends on the HPC machine you are using. For my analysis, I used 2-3 chunks of 3-6 months for each processor setup, giving a total computing time of under a day (running each test sequentially).

Jean-Christophe Rioual: Could a similar framework be used to tune optimally IO servers setup like XIOS ? (with different metrics).

Sergi: It seems possible to me. I don't see why further changes would be needed for the first step of the framework (the prediction script), as I understand that first we want to find the best parallelization for the model and then deal with the IO part. Then regarding the second part of the framework, which originally was intended to reduce the coupling cost by moving processors from one component to the other iteratively, has a pretty standard way of working: 1. run the model, 2. get the perf. metrics and 3. do "something" with them so that the next run is better than the previous. I think that by getting some extra IO-related metrics in the step 2 (probably from the XIOS performance report) and adapting the step 3 so that instead of moving processes from one component to the other could reduce/increase the number of IO servers we may end up with a tool to find the optimal number of servers to use for that model.

Iva Kavcic: Given runtime variability on HPCs, have you got an estimate on how metrics could change between individual simulations? If there are multiple runs, do you use maximum runtimes to derive metrics?

Sergi: I normally run multiple chunks for each individual setup and try to have them running for more than 20 minutes. Then I just average the results from all executions. But for instance, in the ECMWF machine (CCA) I end up running longer experiments as I was observing a high variability (compared to MN4). You must find the right number of tests and runtime for your application/HPC platform by experience and my numbers are for reference only

Kristian Mogensen: Are you worried about run time variability? A HPC machine is a shared resource among many jobs and sometimes e.g. the I/O system can be saturated leading to artificial longer run time for a specific test.

Sergi: Hi Kristian, can you please refer to Iva & Jan's answers

Kristian: Yes. Good answer btw.

Richard Hill: Just a footnote about Kristian's point.. runtime variability is a constant pain when trying to assess performance. Short of running multiple jobs and taking averages are there any better approaches to assessing speed/load balance etc?

Sergi: I do totally agree with that and I'm afraid I don't have any other line of action for that rather than what you just said: running multiple tests and longer runs. In the

end, you can end up knowing how much variability you have in your platform by experience and act accordingly. But double-checking the results is always a good practice :)

Ensemble Simulations with the IPSL climate model - Arnaud Caubel

Kristian Mogensen: Are you going to use PsyClone for OPA on GPU's?

Arnaud : We will use what will be available in the reference version of NEMO to use as efficiently as possible GPUs. When I mentioned that developments were underway in NEMO, I wasn't thinking of a particular development but rather a global work

Rob Jacob: Would like to know more about how you start new ensemble members as you go and kill others based on a scoring function.

Arnaud : after a given period, we use an external tool/script to compute score function depending on the objective (data assimilation, heat trajectories,...). According to the score we select members and we move to the next period and so on..

Jan Streffing: What could be the motivation for killing bad members / part of the variability that your model can produce? I think it is at least a different use of the term "ensemble" compared to a lot of literature.

Arnaud : I agree it is a specific usage of the term "ensemble". I use the term "ensemble" only because many members run in parallel. The application we do here is to select trajectories which go in a direction we target, which is a different protocol from the term usually used.

Kristian Mogensen: If you run many ensemble members in parallel like this are you then worried about node failures since the whole MPI job will fail?

Arnaud : in case of node failure, we have to relaunch the pool of members which is running. So far, we didn't worry more than that about node failure but I agree this is a topic we have to take into account for "ensemble" simulations.

Jan Streffing: Could nudging of e.g. large scales be a faster way to study a certain type of event. e.g. a heat wave instead of waiting for one to evolve?

Arnaud : I am not an expert on this scientific question but I think this approach constrains the model less than in a nudging case.

Iva Kavcic: Q1: I heard that parallel writing with NetCDF is slow. What are the main issues?
Q2: If another coupler is used instead of OASIS for ensemble management, would it need to create the MPI inter-communicators to work with XIOS?

Arnaud : Q1 : Parallel writing is very dependent on the filesystem you use and dependent on the tuning done on the filesystem itself, but in many cases parallel writing is slower than sequential writing. In our case we chose to use sequential

writing thanks to 2nd level of XIOS server. Q2 : Yes, the coupling framework will have to provide the communicator to XIOS.

Session: Coupling Frameworks II

Status Update on BMI core and extensions - Bert Jagers

Sophie V: If the models themselves do not call any API routine, what does it mean in practice to be BMI-compliant?

Bert: The model developer has to implement the BMI API to allow the outside world to call/query the component in the standardized way.

Jean-Christophe Rioual: You support many language bindings, in practice what are the difficulties with assembling a system with multiple runtime (i.e. Julia+Python+C++ etc...)

Bert: The CSDMS group uses Babel developed by LLNL (<https://software.llnl.gov/Babel>) for language interoperability. They use Python as main orchestrator and there are currently few JAVA components in the community. The interoperability between Python-C-Fortran isn't too difficult if the main component is implemented Python. We're still debating at Deltares how to best deal with the Python and Julia codes in toolchains that should be portable and robust for running on any client hardware.

Iva Kavcic: Didn't quite catch what is the risk when supporting passing MPI communicator before the initialise call. What kind of checks are there that everything is initialised and who takes care of it, BMI or a component?

Bert: before the BMI initialize call a large part of the component's memory will not have been initialized, so performing any BMI call will most likely give undefined behaviour. BMI also doesn't require that the component supports the `bmi_set_value` at that time. Furthermore, the infrastructure cannot query the component for the names of quantities that it can exchange at that state. So, the main driver needs to have some inside knowledge concerning the component being called at that stage: does it need an MPI Communicator, and if so what is the name of the quantity that represents the MPI Communicator.

Carsten Lemmen: I have tried passing OASIS-initialized MPI communicator to ESMF, and passing ESMF-initialized MPI comm to OASIS, but have failed. Maybe I did not try hard enough What (@sophie/@rob/@Dan/@Tony) is the status of passing MPI_comm between your (let's assume Fortran) frameworks? – like accepting a split MPI in your `<frameworks>_init` call.

Bert: interesting question for interoperability between infrastructures. Can you run an OASIS coupled model inside an ESMF coupled system ... or the other way around? I know that there have been interoperability experiments in the past, but they may have

only considered porting a single component over from one environment to the other. I expect that at least all infrastructures have to be compiled against the same version of the MPI libraries, and the “child infrastructure” needs to accept that it may not run on all threads, i.e. it shouldn’t rely on MPI_COMM_WORLD.

Sophie: You should have a look at the optional argument “commworld”, last argument of oasis_init_comp API that we introduce in OASIS3-MCT_4.0 (I think):

commworld [INTEGER, OPTIONAL; IN] : optional argument to specify the global communicator gathering the components of the coupled model. If not specified, MPI COMM WORLD will be used as the default communicator to startup. All components of the coupled model must specify the same commworld argument.

But maybe what you need is the other way around (i.e. having the framework transferring a communicator to a sub system and not having the sub-system passing/imposing its global communicator to the framework)

Rob: That might be a case of which language is doing the MPI communicator creation. The C and Fortran created handles aren’t readable by the other language directly.. In Cpl7, Fortran creates the communicators and passes them to Fortran models so not a problem so far.

See https://linux.die.net/man/3/mpi_comm_f2c

Vijay: Just a comment that we pass communicators created in cpl7 (Fortran) to MOAB (C++) seamlessly through the f2c interface. As long as a component can take in a communicator as an argument, the interoperability should work seamlessly. The communications between the components need to happen on their joint communicator though and so someone needs to create these if you want to transfer information back and forth.

Bert: Thank you Rob and Vijay. That is interesting information! I guess we have been lucky so far in the MPI framework that we’ve used since we haven’t experienced issues while transferring MPI communicators between C++ and FORTRAN without converting them. I’ll look for the f2c (and c2f) converters.

C-Coupler3: an integrated coupler infrastructure for Earth system modeling. - Li Liu

Rob Jacob: Which models are using C-Coupler?

Answer (Li Liu): Several Chinese CMIP6 models used C-Coupler, as an option along with cpl7. There are also some forecast models with WRF, ROMS, POM, Mitgcm, Wavewatch, Swan, GRAPES, LICOM, etc. Moreover, C-Coupler3 has been deeply involved in developing a next-generation forecasting system (named MCV) of China Meteorological Administration. Complete paper: <https://gmd.copernicus.org/preprints/gmd-2022-257/>

Iva Kavcic: I am curious about the design of C-Coupler3 given that it handles coupling, IO and halo-exchange library. There are tools which do just one of these tasks. How

interdependent/separate are these three components in C-Coupler3? What about models that would like to use another tool for one of these three tasks, can another tool and C-Coupler3 be used together?

Li Liu @Kavcic: In C-Coupler3, the halo-exchange library, DA framework, I/O framework and integration framework were designed and implemented based on C-Coupler2. All of them utilize existing APIs and configuration files of C-Coupler2 for registering model grids, parallel decompositions and model field instances, while they are independent in usage, with separate APIs and configuration files. C-Coupler3 can cooperate with other couplers or software infrastructures in the same model system.

Moritz Hanke: @Iva: Considering your question, are you not satisfied with the performance of YAXT in LFRic?

Iva Kavcic: @Moritz, yes, we are satisfied, both with the performance and support from YAXT developers when we find issues :-). My question was more on the line of seeing what couplers are out there and can they work with the tools that we're already using in LFRic and know they work (such as YAXT). Also, it seems to me that many couplers do IO and at least one more thing besides coupling and I wonder why not just combine existing tools so to not write everything from scratch :-)

Rob: YAXT?

@Rob: Yet Another eXchange Tool ;-). Computes communication patterns and does data redistribution. Very basic but also very efficient. (<https://dkrz-sw.gitlab-pages.dkrz.de/yaxt/>)

Li Liu @Kavcic: I think there are at least two advantages to develop an integrated coupler platform with various infrastructure supports. First, code base can be minimized, as many infrastructures can reuse existing functionalities of a coupler, especially the data transfer and data interpolation. Moreover, a framework can support the implementation of another framework. For examples in C-Coupler3, the integration framework works as the foundation of the DA framework; the parallel optimization technologies also improve initialization of the halo-exchange library and other frameworks. Currently, C-Coupler3 has less than 73000 code lines. Second, it can provide the same suite of interfaces to simplify the learning curve of various software supports. In China, the responsibilities of our C-Coupler team include not only developing various software products for models, but also applying software products into real Chinese models. As our team is small (no more than five persons), we prefer to develop an integrated coupler platform minimize our work.

Tom Clune: To be fair ESMF also does all 3 of those things. Though I suppose the I/O now delegates to PIO, and was previously not a major focus/capability.

Jan Streffing: What type of control file format does C-Coupler use?

Li Liu @ Streffing: configuration files in XML format.

Carsten Lemmen: What type of changes does your Coupler impose on the model components, keyword "code invasiveness". Just by example, how did you need to change ROMS (or WRF) to be able to be a component in your framework?

Li Liu @ Lemmen: Changes include new code for registering component model, grids, parallel decompositions, field instances and coupling interfaces, and the corresponding configuration files.

SophieV: Yes, C-Coupler design is very similar to OASIS3-MCT

Automating the Coupling Configuration for EC-Earth. - Uwe Fladrich

[UF: Sorry for late answers, I had to jump on the plane right after my talk and was traveling over the weekend.]

<https://github.com/uwefladrich/rdy2cpl>

Jean-Christophe Rioual: There is nothing specific to EC-Earth in your data model of the namcouple, is there ? Could it just be distributed as part of OASIS3-MCT ?

UF: The data model deals exclusively with OASIS, no EC-Earth specifics are involved. And yes, it could be part of OASIS (happy to contribute the code), but it needs some more discussion which form and which features would be most helpful. There is, however, some part of the code that "knows" the grids (regular, general reduced Gaussian, Tco, Tl, ORCAx at the moment). You could consider this a model dependency, but it is written to be extendable in an OO way, so new model grids can be added (add new derived classes).

Sophie: Where does the yaml version of the na,couple comes from? Ec-Earth read the information from that file?

UF: First, I try not to focus too much on the YAML format. It is one (good) option, but the namcouple data model could be created from other formats. Given that, the file has to be provided by the model developer and/or model user. The point is, that both OASIS and other parts of the simulation workflow (such as the model itself) can read it, just as you suggest. So yes, EC-Earth reads the information.

Jan Streffing: Would it be possible to use the examples for test interpolation with your new setup, controlled from the pyoasis? In this case you could get not only OMP and field level but also full MPI parallelization.

UF: I do not fully understand the reference to the "examples for test interpolation". I guess you refer to pyoasis/examples/11-test-interpolation/? Which aspects of the examples therein would you want to use? The interpolation test code in rdy2cpl is based on (two of) the test functions in the benchmarking article, which I think is very useful common ground. Other than that there is the obvious idea of evaluating the test function on the source and target grids, and computing the point-

wise error, which is common. May be I miss a point, please get in touch so we can continue on this point.

Richard Hill: Very interesting (as usual!) and as Jean-Christophe intimates, we're attempting to address similar issues with namcouple generation (based on information entered by model users in a GUI).

UF: Thanks! Good to hear that you are thinking in the same direction, it proves that we really need these workshops even in the future ;-)

For me, the main issue is/was that the data model + Python programming is a game changer when it comes to development of tools. It is just so much easier.

I would be interested in seeing what information/choices you expose to the users by your graphical tool. I always struggle to find the right level of flexibility vs complexity of configuration.

Stefan Poll: Thank you for the talk! Does it need OASIS3-MCT \geq v5.0? Is it possible to manage just passing of one quantity and interpolation by YAML?

UF: Yes, at least OASIS3-MCT5.0 is needed because of pyOASIS. And I do not want to hide the fact that setting up OASIS + Python (and your model) can still be a bit tricky. The good news is that things steadily get better, with better support for virtual environments on HPC systems, for example.

I am not really sure what "passing of one quantity and interpolation by YAML" means. YAML is just used to store the information that ends up in the namcouple data model, it has not any functionality on its own.

XIOS-3 : Toward a new infrastructure of HPC services and model coupling. - Yann Meurdosoif

Jan Streffing: Is the API of XIOS3 backwards compatible with XIOS2.5? Can I swap out the XIOS source code and get the upgrades of XIOS3 without modifications to the interface in my model and rewriting the XML files?

Mainly, yes. Read requires an XML adjustment which will be compatible with XIOS2.

Sophie: Can you give more detail on what you mean by "dynamically schedules ..."

That means the new infrastructure is able to allocate service at any time of the run.

But for now, in the fact, service are allocated at XIOS initialization, but this constraints could be relaxed in future if needed.

Rob: Can XIOS3 work with a second coupling framework? If its controlling mpi-comm-world, I'm not sure.

For now, we validate XIOS3 within IPSL coupling model which runs with OASIS. The coupling framework will have to provide the communicator to XIOS

Andrea: Is the client side library capable of providing some services on local resources?

Yes in attached mode, but we will review how is it currently managed in the next months for better stability and performance. For future service, for example for AI inference, it is important that the service can be running locally, since transfer through the network is a performance killer

Andrea: By which tools or metrics are you estimating memory consumption and potential leaks?

For memory consumption, we are looking at the system (/proc/cpuid....) to get virtual memory, RSS and a max RSS evaluation to catch NetCDF overheads.

Leaks are tracked within the test suite using a dedicated compilation mode (see --memtrack) at build time. This is wrapping memory allocations using the memtrack tool.

Sergi: Can you get the memory consumption metrics only for processes running the XIOS servers or you can get that for the processes running the different components. In case of the latter, could we profile the component's memory consumption?

For all components running XIOS : each call to the XIOS API is monitored.

Yes, we (have to) provide the API to do so. (don't remember if I committed it)

Andrea: Any plan of moving toward git (easier for a community code)?

Yes, of course, very soonly I think...

I hope !

Iva Kavcic: We touched on potential integration of OASIS and XIOS in the future in the Wednesday discussion since XIOS is also looking to implement coupling. My concerns are flexibility and potential overheads if we want to use just one capability, IO or coupling, but not both. Also, that it doesn't want to control the MPI communicator for a model run but plays nicely with other tools that want to use it :-)

Yes this is very important, but be sure that use of such tools concurrently, that manage and split communicators in different components, is a big potential source of problems, and a good orchestration of these from the user is very important to avoid dead-locking.

Jean-Christophe Rioual : With XIOS2.5, spatial and temporal filters are applied on the clients, can we offload them to "servers" with the new XIOS3.0 service architecture ?

Yes, it's one of the idea of the new architecture which should permit to move feature where it's smart to be run. This is the idea to develop an offload service for which you can decide on how much ressource you want to offload a piece of the XIOS workflow, and if you want separate ressources for different diagnostics or the same resource for all offloaded workflows. Flexibility is the key

Tony Craig: Just to be clear, if you don't want to do asynchronous I/O, then XIOS does not need to be launched as a separate component using hardware resources and you can still do all the IO, filters (including mapping), and coupling between models?

Yes, it is independent. You can also use I/O functionalities without servers transparently. You will be synchronous and lose the overlapping of writing and computation. Also, all clients will participate to the writing, which is not very good for parallel file systems.

Rob Jacob: In the mpirun example, the number of mpitasks for servers was larger than the total for the models. Is that typical?

No, it was just a demonstrator for the example. In general, for IO service, about 5% of the whole resources is enough for I/O services (for instance on the NEMO example with a lightweight workflow we used 80 servers for 2688 NEMO process)

Andrea: Moritz is saying right now that YAC moved to YAML input files. Is XIOS staying with XML?

Yes, for now we don't see any reason to migrate. And it may be a problem for retro-compatibility.

Update on YAC and coupled high resolution ICON-ESM - Moritz Hanke

Caroline: Looking forward to the YAML input files ;)

Vijay Mahadevan: I like the visualization tool. We wrote something similar in MOAB for visualizing high-order mapping weights. Are you showing a vector of where each DoF is coming from in the NN method? Does it work in a similar fashion for say bilinear method to show the patch of cells to reconstruct the linear interpolant?

Moritz Hanke: It works for all weight files (if they only have a single source field, but could be extended). But big stencils are hard to interpret in the visualization. (comment by **Carsten**) I remember Ufuk presented a similar Paraview-Catalyst online visualization tool for ESMF/NUOPC at the last Coupling workshop

Vijay Mahadevan: Thanks. Sophie, the MOAB visualization tool can read standard SCRIP maps if you are interested.

Ha Hagemann: in the next released version of the HD model, the python code to visualize the weights that Moritz has mentioned will be included.

Jan Streffing: Are there any users besides ICON already?

Moritz Hanke: HIRHAM-NAOSIM: <https://gmd.copernicus.org/preprints/gmd-2018-278/>

HD <-> ICON (Hydrology model from Helmholtz-Zentrum Hereon)
currently being implemented mHM<->ICON:

<https://www.ufz.de/index.php?en=40114>

in planning: FESOM2 <https://fesom.de/models/fesom20/>

Robert Oehmke: I agree about the visualization! Are those vectors that show the link between source and destination for visualization? (I think I'm asking the same thing as Vijay above, so one answer is fine. :-))

Moritz Hanke: Yes, they are vectors. You can actually color them using the weight itself.

Robert Oehmke: That would be useful for debugging. I'll have to take a look at doing that (or using someone else's) Interesting presentation. Thanks!

Jean-Christophe Riual: Your main application is coupling ICON to ICON, have you considered making the tool more specific to the model - for getting direct access to ICON internal data structures, maybe performance benefits ?

Moritz Hanke: Performance is fine without any specialization.

Iva Kavcic: @Moritz, thanks for the interesting presentation. The performance requirements may change as more users apply YAC on their own grids. Specialisation may be useful in such a case. However, implementing it brings practical issues of code management and how much overlap there is between different "specialisations". My guess is that you don't want to make YAC too big by putting in separate functionality for each grid case. Of course, a user can build an API on top of YAC for such an implementation in their own repositories. The question is then is there something in a user API that would be useful to YAC in general and how to bring that in if so.

Moritz Hanke: Actually, YAC cannot be specialized for any grid... All input grid data is internally converted to an unstructured grid. And internal algorithms depend on this. (However, the interface supports various grid types.)

Iva: Ah, thanks for explaining :-) I'll have a look at the repo to see what exactly you do.

Jan Streffing: Is there a public repository for YAC?

Iva: Good question - I assumed there is but can't find it.

Moritz Hanke: <https://www.dkrz.de/en/services/software-development>
<https://gitlab.dkrz.de/dkrz-sw/yac.git>

Fortran-Python Bridge for Machine Learning Applications in Earth System Models - Caroline Arnold

Joshua Brook-Lawson: How transferable is the training dataset to other cloud physics scenarios?

Caroline: I think the superdroplet scheme is intended for warm rain processes only, to extend it to ice formation etc there would have to be some concept of

thermodynamics. The superdroplet scheme is described here:

<https://agupubs.onlinelibrary.wiley.com/doi/full/10.1029/2020MS002301>

How transferable would this ML method be to apply to a LES climate model? For example to take care of the CFD prognostic equations - momentum, heat, evaporation fluxes etc..?

Caroline: ~~I will pass that question on to my collaborators who are more knowledgeable in climate modeling than I am~~ – The ML method could be applied for cloud microphysics within LES as well, to handle momentum etc it would need to be trained on appropriate data, currently it cannot output values beyond the cloud/rain moments

Iva Kavcic (just to record my question): Are there differences between various ML models that would make coupling difficult and need to be addressed as special cases by your tool? Have you encountered difficulties so far?

Caroline: Both the “embedded Python” and the “YAC” bridge allow the ML users to attach any Python code, so we are not limited with the model architecture. For very large models, it may be better to do the inference on GPU instead of on CPU, but we have not run into that limit yet

Rob Jacob: Did you try SmartSim?

Caroline: Yes we tried SmartSim, but its orchestration would require a rewrite of ICON’s own startup procedure that is beyond our current scope.