IS-ENES3 Deliverable D4.1

Coupling workshop report

Reporting period: 01/07/2020 – 31/12/2021

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Release date: 30/11/2020
CERFACS Technical Report TR-CMGC-20-165

ABSTRACT

The 5th Workshop on Coupling Technologies for Earth System Models (CW2020) was held virtually on September 21st-24th 2020. 152 leading researchers and practitioners in the field of coupling infrastructure for Earth System Models from all around the world registered, and about 80 people attended each session. Five different sessions gathering 35 presentations and an additional 2-hour discussion session were organised to discuss the latest updates on coupling technologies, coupled applications in Earth System modelling, computational performances of coupled models, links between data assimilation and coupling, and coupled model workflows.
This document presents in more details the different themes discussed and conclusions and recommendations that can be drawn from the workshop.

Dissemination Level		
PU	Public	X
CO	Confidential, only for the partners of the IS-ENES3 project	

Revision table			
Version	**Date**	**Name**	**Comments**
Release for review	14/11/2020	Sophie Valcke	
Internal Review	27/11/2020	Richard Hill	
Internal Review	27/11/2020	Uwe Fladrich	

This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No 824084

Table of contents

Executive Summary

The 5th Workshop on Coupling Technologies for Earth System Models (CW2020) was held virtually on September 21st-24th 2020, with one session of 3.5 hours each day. 152 leading researchers and practitioners in the field of coupling infrastructure for Earth System Models from all around the world registered, and about 80 people attended each session. Five different sessions gathering 35 presentations and an additional 2-hour discussion session were organised around the following themes:

- Coupling technology latest developments
- Coupling models in practice
- Computational performances of coupled models
- Data Assimilation and NWP
- Coupled model workflows

Updates on different coupling technologies, i.e. OASIS3-MCT, YAC, C-Coupler2, or MOAB-TempestRemap were presented. Different higher-level coupling layers were also discussed, such as ESM-interface, the MAPL coupling layer, or CMEPS.

The compatibility or "coupleability" of the different coupling technologies was discussed in more detail. One proposed approach would be to define a coupling standard interface and ensure that the different coupling technologies adhere to that standard. A more realistic approach might be to simply accept to develop different higher-level interfaces for each component model, one for each specific coupling software.

Issues related to regridding/interpolation raised high interest. It was proposed to develop a benchmark for comparing the accuracy and performance of the regridding algorithm implementation in the different couplers and a first proposition was put forward.

Details of several coupled applications, assembling the components of the Earth System, were presented. In particular, conservative coupling of river runoff was discussed. The question of dynamic coupling also generated interesting discussions; examples presented during the workshop currently suffer from crude implementation and the coupling infrastructure of these models needs to evolve in order to reinvoke efficiently all needed steps when the model grids or masks evolve.

Different aspects of coupled model performance were discussed, including the importance of running applications with appropriate process and thread affinity for the specific architecture and memory hierarchy of the computer platform used, methods using coupling information to define an optimal load balance of the different components, and the (non-)readiness of couplers to deal with heterogeneous hardware, e.g. CPU-GPU systems.

Four different prediction systems implementing weakly-coupled data assimilation were presented and a more general discussion raised the need to converge data assimilation tools and couplers to minimize duplication of developments. A specific workshop could be organized on this subject, in conjunction with the next Physics-Dynamics Coupling in weather and climate models (PDC) workshop.

Finally, different solutions for managing the coupled model simulation workflow were presented and an interesting discussion dealt with the difficulty of coherently configuring the coupled system, the coupler and the component models, using or not the coupler configuration information as a starting point.

1. General presentation and objectives of the workshop

The **5th Workshop on Coupling Technologies for Earth System Models (CW2020)** was held virtually on September 21st-24th 2020, with one session of 3.5 hours each day. The workshop aimed to bring together leading researchers and practitioners in the field of coupling infrastructure for Earth System Models. This workshop is the fifth in the series[1], started in 2010 in Toulouse and followed by Boulder USA (2013), Manchester UK (2015), and Princeton USA (2017).

152 people from all around the world registered, and about 80 people attended each session. A google document was opened for questions. People were encouraged to write down questions and remarks during the talks. Some questions were answered directly during the presentation by other participants, leading to fruitful interactions between the workshop attendees. At the end of the talk, the session chair summarised the remaining questions during the 5-minute question period. If there was not enough time to answer all questions, the speaker could do so afterwards in the google doc. At the end of the workshop, this google document is 48 pages long!

2. Workshop agenda

Five different sessions gathering in total 35 presentations were organised around the following themes:

- Coupling technology latest developments
- Coupling models in practice
- Computational performances of coupled models
- Data Assimilation and NWP
- Coupled model workflows

The complete program is available in Appendix A.

An additional 2-hour session was organized on the Monday following the workshop as participants felt there were still many issues to discuss further. The subjects discussed were the following:

- compatibility or “coupleability” of the different coupling software
- implementation of the regridding in the different couplers, in particular the conservative remapping
- the readiness of couplers to deal with heterogeneous hardware, e.g. CPU-GPU systems
- the relation between data assimilation tools and couplers

Developers of different coupling software and coupling infrastructures participated in these additional discussions, which resulted in very rich exchanges.

[1] https://portal.enes.org/community/community-workshops/

3. Overview of sessions and discussions

We provide here an overview of the coupling software, coupled applications and coupling issues presented and discussed during the workshop in the different sessions planned in the agenda and in the additional session that took place on the Monday following the workshop. We will not go through a chronological description of the sessions as the subjects addressed often overlapped; instead we will try to give a summary of the presentations and related discussions grouping them per subject.

3.1 Coupling technologies and higher-level coupling layers

Different coupling technologies were presented during the workshop. As already observed, coupling technologies can be broadly classified into two prominent categories, i.e. the "external coupler or coupling library", and the "integrated coupling framework". In the first approach, illustrated by presentations on OASIS3-MCT, YAC, C-Coupler2, or MOAB-TempestRemap, the component models remain separate executables and the original codes are modified as little as possible; the component codes are instrumented with calls to the coupling library Application Programming Interface (API) and the synchronization of the components is implicitly ensured by the coupling exchanges. The "integrated coupling framework", for which ESMF/NUOPC is a quintessential representative (but also FMS at GFDL[2] or CPL7 at NCAR[3], not presented at the workshop) involves splitting the original component codes into initialize, run and finalize units, adapting these units to standard data structures and routine interfaces, and rebuilding a single integrated application based on these units, with a top-level driver controlling the component execution. Updates on the different couplers including details on their regridding/interpolation functionality, their community and applications, were presented.

Different higher-level coupling layers were also discussed, such as ESM-interface, a coupling interface to both OASIS3-MCT and YAC, the MAPL ESMF-based coupling layer within the GEOS (Goddard Earth Observing System) data assimilation system, or CMEPS (Community Mediator for Earth Prediction System) that is the new NUOPC-compliant coupling architecture of the NCAR Community Earth System Model (CESM). OBLIMAP, a specific regridding package for coupling general circulation models and ice sheet models was also presented.

These presentations prompted significant interaction between participants on various issues. Examples are use of ESMF remapping for NEMO grids and their specific North fold, the recent interfacing of MOAB in ESMF, the impact of non-matching sea-land masks in the ocean and the

[2] https://www.gfdl.noaa.gov/fms/
[3] https://www.cesm.ucar.edu/models/cesm1.0/cpl7/

atmosphere, cost of data transfer for implicit coupling and how the FMS/GFDL approach precludes the need to transfer 3D fields.

"*Coupleability" of the different coupling software*

A specific issue, the compatibility or "coupleability" of the different coupling software, was discussed in more detail. Potential use cases are, for example, an ESMF coupled system containing an OASIS3-MCT-coupled application; or simply coupling one component interfaced with OASIS3-MCT with an ESMF/NUOPC-compliant component.

One solution presented at the workshop is the design of a higher-level interface to different couplers, like the esm-interface used for YAC and OASIS3-MCT. However, that approach may work only for couplers with the same design philosophy and would probably be much harder to implement between couplers belonging to the "external coupler or coupling library" and "integrated coupling framework" categories (see above).

BMI (Basic Model Interface), which is an attempt to define a standardized interface to geophysical model functions (e.g. control, time, grid), is another approach to compatibility of models in general. This should be considered as a potential means to define standard coupling interfacing. However, it was also mentioned that the required standardization of the coupler APIs may be impossible to achieve as the different coupling software addresses different coupling requirements and, again, follows different design philosophies. It was reported that there have been previous attempts to build generic coupling interfaces but most of them have been broken by additional specific requirements or use cases.

A more pragmatic approach might be to simply accept the need to develop a different interface, or "cap", to a specific coupling software. Although difficult to achieve in practice, effort would be made to reduce the total development effort and the number of couplers available by merging the ones that offer the same functions and follow the same design philosophy. These two approaches can also be seen as complementary since closer standardization of APIs would result in reduced complexity for the different caps.

Coupling software regridding functionality

Issues related to regridding/interpolation were heavily discussed, such as the interesting concept of interpolation stack (user-controlled layering of methods) implemented in YAC, new interpolation capacity in the ATLAS library developed at ECMWF, or the standardization of interpolation weight file format for flexible reuse. Interest was also expressed for better support of vector remapping by the coupling software.

Details were also shared on the implementation of the regridding in the different couplers, in particular the conservative remapping. It was interesting to realize that the 2nd order conservative remapping in XIOS, YAC and ESMF is based on the same algorithm described in Kritsikis et al 2017. MOAB-TempestRemap includes a special scheme based on an advancing-front intersection algorithm and a resulting "supermesh" based on the source and target grids.

It was also proposed to develop a benchmark for comparing accuracy and performances of regridding implementation in different couplers. A first proposition was put forward detailing mesh representations, field representations, algorithms for neighborhood search and edges intersections, types of regridding supported, safeguards on the remapped fields to be covered in the comparison (see https://drive.google.com/file/d/1WgGUlJpBLrtbI_fnUOdfNiGx98E7d89N). Metrics were proposed to evaluate the sensitivity (algorithmic invariance to underlying mesh topology), conservation, consistency (preservation of discretization order and accuracy), monotonicity (preservation of global solution bounds), and performances of the library, based on the CANGA-ROO project. Various coupling software developers present expressed interest in participating in such a benchmark.

3.2 Coupled applications

Several talks on different applications coupling the different components of the Earth System, i.e. ocean, atmosphere, sea-ice, land, as well as ice sheet, biosphere or coastal ecosystem constituents, were presented, for example:

- the US Navy Earth System Prediction Capability (Navy-ESPC), a global coupled atmosphere-ocean-sea ice prediction system ;
- the Unified Forecast System (UFS), the NOAA community-based operational weather and environmental modeling system ;
- the atmosphere-biosphere-land coupled system developed at the National Institute of Technology in India ;
- the ocean-wave-atmosphere coupled model developed at the "Laboratoire de l'Atmosphère et des Cyclones" (LACy) in La Réunion for the prediction of tropical cyclones ;
- EC-Earth4, a European community Earth System Model ;
- the ocean-atmosphere model ICON-GETM, used at the Leibniz Institute for Tropospheric Research to study local processes over the Baltic sea ;
- TerrSysMP, the Terrestrial System Modeling Platform, coupling the ICON atmosphere model and the Community Land Model at the Juelich Research Center ;
- MOSSCO, the coastal ecosystem coupling physical, biogeochemical, ecological and geological processes at the Helmholtz-Zentrum Geesthacht center ;
- the ocean-sea-ice model assembling NEMO and neXtSIM, a sea-ice model using a Lagrangian moving mesh to better simulate the discontinuities in sea-ice properties;

- UKESM1, the Earth System Model developed in the UK, including in particular an interactive ice sheet model.

Runoff coupling

Details on how to conservatively couple runoff in global climate models were also introduced. It was noted that this type of coupling has a reverse rationale compared to other couplings, in the sense that the aim is to make sure that all source grid points discharge their runoff in at least one target grid *point*, whereas the usual rationale is to make sure that each target point gets one meaningful value. Different conservative methods with horizontal and/or vertical spreading of the different fluxes were evoked.

Dynamic coupling

The talks on the sea-ice model using a Lagrangian moving mesh and on the interactive ice sheet model generated interesting discussions related to dynamic coupling. Currently these coupled models suffer from crude and sub optimal implementations. In some cases, the impact of the evolution of the coupling characteristics (e.g. the ocean solid boundary and 3D grid due to the advance/retreat of the ice sheet) can be currently handled only by restarting the coupled model. This is linked to the need to recalculate the regridding weights but also, for example, to the impact on the ocean topography. In other cases, the coupling with the moving grid is done through a fixed grid in order to minimize the difficulties linked to a constantly changing spatial partitioning. The coupling infrastructures of these models need to progress and improve in performance in order to reinvoke efficiently the steps needed when the model grids or masks evolve.

3.3 Computational performances of coupled models

A few talks, reaching a high level of technical expertise, discussed the cruciality of running an application with proper process and thread affinity, given the specific architecture and memory hierarchy of the computer platform used, for efficiency and performances. It was noted that the question is even more complex for our climate coupled applications where the different components can have different ratios between MPI processes and (possibly nested) OpenMP threads, or where this ratio may have to evolve at runtime given the different tasks to chain (e.g. the same processes may be initially calculating the regridding weights and then running a component model per se). It was observed that the question of how to optimally map the coupled application on the available resources is a delicate and often platform-dependent issue. Tools, such as HIPPO and Quo, that dynamically rebind processes and threads to match the different phases of an application with calls from within the application code, were introduced.

Tools to help manage the complexity of coupled models on different architecture (e.g. CANGA by Los Alamos Lab) were presented. Methods to define an optimal use of available resources and an optimal load balance of the different components, based on performance metrics calculated by the coupler during a coupled run were also discussed and compared with the possibility of using more complex profiling tools as Extrae/Paraver.

Another question specifically addressed was on the readiness of couplers to deal with heterogeneous hardware, e.g. CPU-GPU systems. Although some thinking is going on, this issue has not properly been addressed yet in most couplers, at least not in OASIS3-MCT and not in ESMF. Some doubts were raised about the use of GPUs for couplers given their relatively small compute load, but the potential role of GPUs for offline regridding weights generation could be considered, even if currently MPI parallelism yields excellent speed-up. In all cases, coupling infrastructure working with top-level drivers should be aware of GPU resources so as to appropriately allocate resources to the different components. In fact, an abstraction layer called VM was developed for ESMF to add the ability to map different components onto the available resources, including GPUs if available.

3.4 Data Assimilation (DA) and Numerical Weather Prediction (NWP)

At least four different prediction systems implementing weakly coupled data assimilation (i.e. performed in each component separately) were presented during the workshop:

- At the UK Met Office, the system is based on the Unified Model atmosphere, the JULES land surface, the NEMO ocean and the CICE sea ice models; plans are to start using this coupled model for operational NWP from autumn 2021.
- ECMWF has a weakly coupled data assimilation including waves, land, ocean and sea ice components. The impact of a change in one part of the DA system on the other parts of the DA system, given the different timescales of error growth, was discussed, highlighting the fact that the complexity of ESMs can be a significant barrier to their use in operational DA systems.
- The system at Environment and Climate Change Canada system is built on four independent atmospheric, ocean, SST and sea-ice data assimilation components; only the atmospheric and ocean data assimilations are weakly coupled, i.e. share common model background states from the coupled atmosphere-ocean model to compute two independent analyses.
- The Navy Earth System Prediction Capability (Navy-ESPC) global coupled model is based on the Navy’s Global Environmental Model (NAVGEM) for the atmosphere, Navy’s HYbrid Coordinate Ocean Model (HYCOM) for the ocean, and the Los Alamos National Laboratory’s sea ice (CICE) for the sea ice.

A presentation on Ensemble Data Assimilation for Earth System Models based on the Parallel Data Assimilation Framework (PDAF) raised specific discussion on interactions between the coupler used within the ESM and the infrastructure used for the DA; in the present case, PDAF bypasses the coupler and questions were raised about the risk of duplicating functionalities.

A more general discussion addressed the relation between data assimilation tools (like OOPS, JEDI, PDAF, Open-PALM) and couplers and, more generally, between data assimilation systems and coupled applications. It was mentioned that some integrated coupling frameworks already include data assimilation functionality, like FMS. It was observed that in general, the infrastructure used for coupling has been developed independently than the infrastructure used for DA and it would be relevant to start converging these two in order to minimize duplication of similar developments like interpolation. A specific workshop could be organized on this subject. Another option is to organize a specific common session on this subject at the next Physics-Dynamics Coupling in Weather and Climate Models workshop (PDC, see https://pdc-workshop-abstracts.com/event/2) planned in June 2021. The possibility of organizing back-to-back workshops between PDC and the current series of Coupling Workshops is envisaged for fall 2022 and that special session could then be organized.

3.5 Coupled model workflow

Many different solutions for managing coupled model simulation were discussed in different sessions during the workshop, which indicates that model coupling and workflow are two intricated issues:

- The eWaterCycle platform offers an integrated environment for hydrological modelling;
- ESM-Tools is a collection of scripts to download, compile, configure, and run different Earth system simulations;
- OMUSE is a Python environment for numerical experiments in oceanography and other climate sciences including, in particular, model setup and runs, run control, online data analysis, ensemble simulations and model comparison;
- The EC-Earth4 workflow environment relies on different tools (CPLNG, ScriptEngine, Autosubmit, ocp-tool) to manage the different steps in the workflow (development, build, configure, run, monitor, postprocess);
- The IPSL workflow (and also CNRM-Cerfacs'one) has the particularity of using the XIOS IO server together with dr2xml, a package for translating a CMIP Data Request into XIOS configuration files, to directly produce CMIP6 publication-ready data files;
- CESM and E3SM are using the python-based CIME Case Control System.

An interesting discussion dealt with the difficulty of coherently configuring the coupled system, the coupler and the component models, as the coupling information is often duplicated in different places. The question of whether or not using the coupler configuration file (e.g. the *namcouple* for the OASIS coupler) as the starting point was raised. This is the current choice at the Met Office but a new brand control mechanism is currently being developed for next generation modelling systems where the component configuration would generate the coupler control file.

4. Conclusions and Recommendations

The 5th Workshop on Coupling Technologies for Earth System Models (CW2020) gathered leading researchers and practitioners in the field of coupling infrastructure for Earth System Models from all around the world. Five different sessions gathering 35 presentations and an additional 2-hour discussion session were organised and about 80 people attended each session. The latest updates on coupling technologies, coupled applications in Earth System modelling, computational performances of coupled models, links between data assimilation and coupling, and coupled model workflows were discussed. These presentations raised a lot of interest and interaction between participants on different issues. A google document was opened for questions and answers; at the end of the workshop, this google document is 48-pages long!

In general, the community would like to see a reduction in the number of couplers available, by merging the ones that offer the same functions and follow the same design philosophy. |Given the number of existing coupling technologies, their compatibility is an issue that should be addressed. One proposed approach is to define a coupling standard interface and ensure that the different coupling technologies adhere to that standard. A simpler and probably more realistic approach is to simply accept to develop for each component model different higher-level interfaces, one for each specific coupling software. These two approaches can be considered complementary as closer standardization will result in less complex higher-level interfaces.

The implementation of the regridding in the different couplers, in particular the conservative remapping, raised a lot of interest. It was noted that the 2nd order conservative remapping described in Kritsikis et al 2017 is implemented in at least 3 couplers and shows promising results. It was proposed to develop a benchmark for comparing the implementation of the regridding algorithms in the different couplers and a first proposition was put forward. This effort will have to be taken forward by the coupler developers.

The questions of dynamic coupling and coupled model performances also generated interesting discussions. Coupling technologies always need to evolve to efficiently answer the new needs of the community, such as dynamic coupling, and to adapt to the new computing environments. In particular, couplers need to ensure (or at least be compatible with) a proper execution of the component models with respect to process and thread affinity given the specific architecture and memory hierarchy of the computing platform. Methods using coupling information to define an optimal load balance of the different components were presented. The discussion also showed that more reflection is needed on how couplers could exploit new heterogeneous hardware, e.g. CPU-GPU systems; some doubts were raised about the use of GPUs for couplers given their relatively small compute load, but the potential role of GPUs for offline regridding weights generation could be considered.

Regarding data assimilation, it was proposed to organize a specific workshop, in conjunction with the next Physics-Dynamics Coupling in weather and climate models (PDC) workshop, on data assimilation and coupling software infrastructures, in order to minimize duplication of developments and ensure compatibility.

Finally, the workshop showed that many different solutions exist for managing the coupled model simulation workflow. Again, the community should aim at more software sharing on this aspect of workflow management, in order to reduce the total development effort and minimise duplications.

Given the fact that CW2020 was organised virtually, we envisage the possibility to organise the next Coupling Workshop before the end of the IS-ENES3 project. The possibility of organizing back-to-back workshops between the Physics Dynamics Coupling series in weather and climate models and the current series of Coupling Workshops is therefore envisaged for fall 2022.

5. References

Kritsikis, E., Aechtner, M., Meurdesoif, Y., and Dubos, T.: Conservative interpolation between general spherical meshes, Geosci. Model Dev., 10, 425–431, https://doi.org/10.5194/gmd-10-425-2017, 2017.

6. Web links for tools and coupled applications

ATLAS: https://confluence.ecmwf.int/display/ATLAS/Atlas

BMI: https://bmi-spec.readthedocs.io/

C-Coupler2: https://gmd.copernicus.org/articles/11/3557/2018/

CANGA-ROO : https://github.com/CANGA/Remapping-Intercomparison

CESM: http://www.cesm.ucar.edu

CIME: https://e3sm.org/resources/tools/other-tools/cime/

CMEPS: https://github.com/ESCOMP/CMEPS

CPL7: https://www.cesm.ucar.edu/models/cesm1.0/cpl7/

E3SM: https://e3sm.org

EC-Earth : http://www.ec-earth.org

ESM-interface: https://www.esm-project.net

ESM-Tools: https://www.esm-tools.net/get-esm-tools/

ESMF: http://earthsystemmodeling.org

eWaterCycle: https://www.ewatercycle.org

Extrae: https://tools.bsc.es/extrae

FMS: https://www.gfdl.noaa.gov/fms/

GEOS: https://gmao.gsfc.nasa.gov/GEOS/

HIPPO: https://cerfacs.fr/wp-content/uploads/2019/06/Globc-WN-Maisonnave-oasis_hippo-2019.pdf

JEDI: https://www.jcsda.org/jcsda-project-jedi

MAPL: https://dl.acm.org/doi/abs/10.1145/1297385.1297388

MOAB-TempestRemap: https://gmd.copernicus.org/articles/13/2355/2020/

MOAB: https://press3.mcs.anl.gov/sigma/moab-library/

MOSSCO: http://www.mossco.de

Navy-ESPC: https://agupubs.onlinelibrary.wiley.com/doi/abs/10.1029/2020EA001199

NUOPC: http://earthsystemmodeling.org/nuopc/

OASIS3-MCT: https://portal.enes.org/oasis

OBLIMAP: https://github.com/oblimap/oblimap-2.0

OOPS: http://www.data-assimilation.net/Events/Year3/OOPS.pdf

OpenPALM : http://www.cerfacs.fr/globc/PALM_WEB/

Paraver: https://tools.bsc.es/paraver

PDAF : http://pdaf.awi.de/

QUO: https://github.com/lanl/libquo#citing-quo

TerrSysMP: https://www.terrsysmp.org

UFS: https://vlab.ncep.noaa.gov/web/environmental-modeling-center/unified-forecast-system

UKESM: https://ukesm.ac.uk

XIOS: http://forge.ipsl.jussieu.fr/ioserver/wiki

YAC: https://dkrz-sw.gitlab-pages.dkrz.de/yac/

7. Appendix A – Coupling Workshop Program