2020 OASIS3-MCT Development Plan

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1. Context, longer term and funding

OASIS development started in 1991 in Cerfacs. The current version of the coupler, OASIS3-MCT (Craig et al. 2017), offers fully parallel regridding and distributed exchanges of the coupling fields, thanks to MCT (Model Coupling Toolkit, <u>www.mcs.anl.gov/mct</u>) developed at Argonne National Laboratory in the USA.

In 2019, a survey was performed among OASIS users. Each group or person who downloaded the OASIS3-MCT sources since its first release in September 2012 was asked about their effective use of the coupler. This survey confirmed that OASIS3-MCT is used by at least 67 modelling groups to assemble more than 80 different coupled applications over the 5 continents. These applications include global or regional configurations of ocean and atmosphere models but also sea ice, sea level, wave, ocean biogeochemistry, land, vegetation, river routing, hydrological and atmospheric chemistry models. OASIS3-MCT is used in 5 of the 7 European Earth System Models participating to the 6th Coupled Model Intercomparison Project (CMIP6) that produces the climate simulations forming the basis of the next report of the Intergovernmental Panel on Climate Change (IPCC)"

The latest official release of the coupler, OASIS3-MCT_4.0, was distributed in July 2018 (Valcke et al 2018a). OASIS3-MCT_4.0 sources were downloaded about 500 times since its release from groups all over the world. The next release, OASIS3-MCT_5.0, is planned for December 2021. As written above, OASIS3-MCT offers fully parallel regridding and distributed exchanges of the coupling fields. OASIS3-MCT_4.0 includes in particular a hybrid MPI+OpenMP parallelisation of the SCRIP library (previously fully sequential), which shows a reduction in the remapping weight calculation time by 2 or 3 orders of magnitude as compared with the sequential version for high-resolution grids (Valcke et al. 2018b). OASIS3-MCT_4.0 also includes other developments offering a significant gain in performance such as a new communication method based on the remapping weights or new reproducible methods for the global CONSERV operation.

Over the 2019-2022 period, the funding for development is covered by CNRS (0.5 FTE), Cerfacs (0.5 FTE), the IS-ENES3 EU project (12 pms for support and 29 pms for development) and the ESiWACE2 CoE (4 pms for support and 6 pms for development). CNRS and Cerfacs involvement in OASIS can be considered stable; it ensures active user support to the community and the maintenance of the actual code with the possibility of minor upgrades. Additional developments require additional funding as is currently ensured by IS-ENES3 and ESiWACE2. On the longer term, Cerfacs commits to keep on seeking such additional funding and to lead OASIS sustainability effort currently being actively discussed within ENES, as for other ENES services.

Given the latest performance improvements and evolutions proposed in this document, we consider that OASIS3-MCT provides and will keep on providing an efficient and easy-to-use coupling solution for many climate modelling groups for at least the next 5 years.

At the 5-10 year horizon, the convergence with XIOS, the I/O server developed at IPSL, remains under consideration. XIOS is used in many European climate components and includes basic coupling functionality i.e. communication and regridding of data. Indeed, a first 2-way coupling test case with XIOS was realised mid-2020. The convergence between OASIS3-MCT and XIOS was studied in detail in ESiWACE (Valcke et al. 2018c). The analysis lead to the conclusions that 1) XIOS in principle contains most of the functionality required to act as a coupler and 2) that merging the two tools would not be a practical way forward as the effort of merging would be higher than the effort of extending XIOS to include all OASIS3-MCT functionalities, and 3) that it is too early to decide if the convergence should happen as the coupling functionality in XIOS is not fully developed, tested and validated yet. Only if proposed steps, including more development and testing, were successfully achieved, we would then be confident that XIOS can be considered as a candidate for a community coupler.

The ATLAS library developed at ECMWF could also, on the longer term, be considered as a coupling library to promote at the community level. A first analysis of ATLAS as a possible complement to the SCRIP library in OASIS3-MCT in terms of remapping functionality was recently performed at Cerfacs (Piacentini 2020). The conclusion is that the ATLAS design is certainly appealing and can provide a useful portable toolkit for the best usage of new heterogeneous architectures. Nevertheless, its usage as a software foundation for the remappings in OASIS3-MCT in the short term cannot be recommended. Some basic capabilities are still missing, in particular the handling of missing/masked values and the whole chapter of conservative interpolations.

This plan is an evolution of the development plan presented in 2019 (Valcke et al, 2019) based on the experience and analysis of the current OASIS developers and on a user survey realised in 2017, which served for the previous development plans and which details can be found on the OASIS web site¹. In section 2., we present the developments planned for OASIS3-MCT_5.0 due December 2021. All these developments have high priority. For each development, we specify if it is funded by IS-ENES3 (IS3) or by ESiWACE2 (ES2). In section 3, w e describe other developments with lower priority that c ould be considered on the longer term. A specific discussion with the Advisory Board will be organised on these issues after OASIS3-MCT_5.0 is released.

2. Developments planned for OASIS3-MCT_5.0

The developments that we plan to include in OASIS3-MCT_5.0 are described here. As for the previous development plans, they are classified into 5 categories: Interpolation & transformations, Communication, Configuration, Other functionalities, Support & training. We don't list here bugs that are regularly reported and fixed. For each development, we also provide an estimate of the complexity to address it, C1 - being

¹ See <u>https://portal.enes.org/oasis/users/oasis-governance</u>.

relatively easy- up to C4 -being very complex. In most cases, the development is described in a ticket on the OASIS Redmine site (https://inle.cerfacs.fr/projects/oasis3-mct), and we provide the corresponding ticket number. We note also that some of these developments are already completed as we have of course started the work since the release of OASIS3-MCT_4.0 in July 2018; when this is the case, it is indicated with "(done)" in the task title.

Interpolations & transformations

• Interfacing with a high-quality parallel library for the calculation of the regridding/interpolation weight-and-address file, C4, IS3, tickets #2349 & #1011

As written above, the SCRIP library was parallelized with OpenMP/MPI leading to great reduction in the calculation time of the remapping weights. But the SCRIP still shows specific problems near the pole for some grids (Jonville et al, 2018; Jonville & Valcke, 2019; Valcke& Piacentini, 2019) and some algorithms and this motivates the investigation of other parallel interpolation libraries of higher quality. ESMF, XIOS, ATLAS, YAC, MOAB/TempestRemap are considered. This is one of the main tasks funded in IS-ENES3 and the choice will be further discussed with the OASIS Advisory Board. In all cases, the idea is not to replace the SCRIP library but to extend the current mapping options in OASIS3-MCT. The SCRIP algorithms will still be available and remapping weights using the SCRIP format will still be supported

• Conservative remapping for the runoffs, C3, IS3, ticket #2556

When coupling "traditional" fluxes, the basic idea is to provide data on each unmasked target grid point. In the case of river outflow, the rationale is reversed since not all ocean target grid points will receive a value but it is necessary that all source grid points find a target on the ocean grid. The method proposed by Aurore Voldoire at CNRM is based on the regular interpolation weights but taking the reverse interpolation links. This method allows to conserve the river outflow locally and globally and will be implemented in the next version of the coupler. The method supposes that, as for the SCRIPR/CONSERV and the global CONSERV, the runoff is expressed as an extensive property (e.g. in m/s).

• Improved and additional diagnostics, C2, IS3, ticket #2356, #1761 and #1069

Diagnostics, that are currently performed when the CHECKIN/CHECKOUT operations are specified in the *namcouple*, have to be revised as well as how their results are printed in the debug files. The diagnostics that should be performed on the source and target grids are the minimum, maximum, mean, integral and area-weighted integral value. Masks and fractional areas must be considered.

• Pre- and post-processing transformations, C3, IS3, ticket #2364

This task is about extending the current pre- and post-processing transformations (BLASOLD/BLASNEW) with possibly user-defined transformations or combinations with other fields than the coupling fields. We still have to evaluate the cost/benefit of such developments. It would probably be very complex to develop in OASIS3-MCT some general treatment that would cover all possible use cases. Furthermore, we think that in most cases, those specific transformations can be easily coded in the models themselves. We also mention that we think that user needs with respect to this functionality are low, as nobody answered the mail and reminder that were recently sent on the OASIS user mailing list about their corresponding requirements.

• Normalisation by the "true" area for the conservative remapping, C2, IS3, ticket #<u>1010</u> (done)

To be truly conservative the remapping weights have to be normalised by the "true" area of the grid cells i.e. the area of the cells as considered by the models themselves and not as calculated by the remapping library. This option is now available on the trunk version.

- Other issues requiring only minimal efforts, C1
 - Adding the number of neighbours used in the remapping file name so to avoid confusion when the same interpolation is used between the same grids but with different number of neighbours, IS3, ticket #2350 (done)
 - Easy detection of the target grid point that do not receive any value, IS3, ticket #731 (done)
 - Making OASIS3-MCT conformant with CMIP6 standard for weight file format, IS3, ticket <u>#2401</u>
 - Allow the definition of north_thresh and south_thresh values (Lambert projection) through the *namcouple*, IS3, ticket #2459 (done)

Communication

• Extension of the oasis_get_intracomm API routine to support multiple components, C2, ES2, ticket #<u>2687</u>

The API routine oasis_get_intracomm merges two MPI communicators from two different components to form a new communicator. It is proposed to extend this to more than 2 components by overloading the interface. This is needed in coupled models involving both OASIS3-MCT and XIOS when XIOS manages ensemble simulations.

• Sending/receiving simple scalars, C2, IS3, ticket <u>1937</u> (done)

This functionality, i.e. exchanging few scalar values once during the simulation, was asked by few users and is now available on the trunk version.

Other functionalities

• Further development of LUCIA, the load balance analysis tool, C3, IS3, tickets #2357 & #1003

LUCIA is the tool delivered with OASIS3-MCT to automatically evaluate the load balance of the coupled components. Currently the LUCIA analysis only provides information integrated during the whole simulation. A timeline will be made available to better identify load imbalance at every coupling time step. Fully integrating LUCIA analysis tool in the OASIS3-MCT finalisation step (instead of having to run if afterwards) and unifying LUCIA and the standard OASIS timer result presentation is also planned.

• Python bindings, C3, IS3, ticket #2362 and #2509

This is included in the list of developments for IS-ENES3. Python bindings will allow the coupling of models written in Python. It will bring OASIS to a much wider ecosystem and be a good way to attract countries less advanced in HPC. It will be also of great interest when using OASIS3-MCT as an offline interpolator. This will require an update of the compiling environment.

• Analyse and optimise the memory use in OASIS3-MCT, C2, ES2, ticket #1104

Even if there is currently no memory problem reported by the users, it is proposed to run some diagnostics to precisely evaluate the memory consumption in OASIS3-MCT.

• Develop, maintain, and systematically apply the buildbot test suite, C3, IS3, ticket #232

The builbot suite is an automatic testing system composed of more than 20 toy models that are run automatically over three different platforms each time a source is committed in the GIT source manager. The results are automatically analysed and compared to a reference state to detect any bug that would be linked to the new development. We recently revised the suite to make sure that we are testing every important aspect of OASIS3-MCT functionalities. On the longer term, we could envisage switching to unit tests (instead of using toy models) but this would be a big step change. We consider with high priority the maintenance and further enhancement of the current test suite.

• Format of files for EXPOUT coupling field, C2, IS3, ticket #2365

When written out for debug, each bundle member appears in a different file. Some users have reported that they would find it more practical to have all bundle members into one file. Other users would like to have the field grid written out in debug file for easier plotting.

• New API interface for oasis_def_var, C2, IS3, ticket #2273 (done)

One argument of oasis_def_var is not used anymore but is mandatory for backward compatibility. A new interface has been defined without the unused argument and both the old and new API are supported. This feature is now available on the trunk version.

• Systematic tests of NetCDF returned error code, C2, IS3, ticket #550 (done)

Support and training

It is also very important for us to keep on offering high quality user support and training, in particular (in order of priority from the highest to the lowest):

- Regular user support through the forum, by mail or by phone, C2, IS3
- Training, C3, ES2

Training on OASIS3-MCT will continue to be offered on a regular basis. In the current sanitary context, on-line training will be preferred until face-to-face training can resume. A SPOC (Small Private Online Course) has been recently developed in the framework of ESiWACE2(see https://cerfacs.fr/code_coupling_with_oasis3-mct/). This SPOC will be enhanced with additional exercises and will be officially delivered at least twice a year. The next session is planned April 19th-25th 2021.

• Dedicated User Support, C3, IS3 & ES2

Dedicated User Support, i.e. organising the visit of an OASIS developer to a chosen institute to help setting up or optimising a coupled system, is provided in the IS-

ENES3 and ESiWACE2 contexts with respectively 9 pms and 4 pms. In 2019, the support was provided as planned. In 2020, the support has suffered some delay due to covid-19 but we are still planning to provide the total level of services planned before the end of those two projects.

• Toy coupled models, C2, IS3, ticket #2555 and #2175

A toy coupled model coupling a fake atmosphere model and a fake ocean model is delivered with the coupler sources so that users can get familiar with compiling and running with OASIS3_MCT. This toy coupled model has been revised while developing the SPOC and will be made available to the users with the next official release.

Another toy model showing how a vector field should be coupled will be developed. In that case, the source component of the toy must project the original vector field on a cartesian space and send the 3 projected components. The target component receives the 3 components (on the cartesian grid) and must project them on its grid and verify that the resulting vertical component is null.

• Environment to create fractional areas for truly conservative remapping, C2, ES2, ticket #2460

In an ocean-atmosphere coupling, the binary (i.e. not fractional) ocean mask should be taken as it is from the model. For the atmospheric model, coupling cell fractions should be defined by the conservative remapping of the ocean mask on the atmospheric grid, retaining fractions above a certain threshold. These coupling cell fractions should be used in the atmospheric model to define the % of ocean subsurface to be considered. Then the atmospheric coupling mask should be adapted associating a non-masked index to all cells with an ocean fraction above the chosen threshold. An environment reproducing all these steps will be developed and made available to the users.

• Migration from SVN to GIT for source management, C3, IS3, ticket #2352 (done)

Using GIT for source management is of great benefit for the OASIS3-MCT users, in particular, given its distributed method for version control, which means that each user clones a full version of the repository to her local machine. GIT branching and merging features are also more evolved than in SVN.

3. Other longer-term developments

Interpolations & transformations

• Dynamic weight calculation for dynamic grids, C4, ES2, ticket #2400

Supporting coupled applications including components with grids having a mask evolving with time will be considered (after OASIS3-MCT_5.0 release). Examples of coupled systems including dynamic masks exist, e.g. ice sheet or sea ice models. As a first step, dynamic masking via weighted mapping capability (no extra weights generation per se needed) will be considered. In the longer term, adding the capability to map in parallel the fields expressed on a dynamic grid to a static coupling grid could be envisaged.

• Vertical interpolation, C4

Simple level-to-level or pressure-to-pressure interpolation would be relatively simple to implement but more sophisticated pressure-to-level or hybrid-to-level would be much more complex (because the interpolation then depends on auxiliary field that changes at each coupling timestep). We consider that this is better done in the model themselves and give only a low priority to that task.

Configuration

• Modernisation and extension of namcouple syntax, C3

The priority of this task is debatable. We have considered transforming the namcouple format (xml, yaml, standard FORTRAN namelist). Finally, we have always come back to the conclusion that the current ASCII format, even if not extremely friendly, fulfils its mandate and changing it, while keeping the same quality of error handling, would require a non negligible effort and maybe other external libraries, for low benefits.

• Layer for "automatic" configuration of the coupling exchanges in the models based on the namcouple, C3, in ticket #2361

The idea is to define, in the namcouple, a unique identifier for each coupling field. The identifier would have to be associated to a coupling field array in the model but, besides this, all coupling actions would be automatic.

Other functionalities

• Support of heterogenous hardware, e.g. CPU-GPU systems, C4

This issue has not properly been addressed yet in OASIS3-MCT but will have to be, given the evolution of the computing platforms. Although couplers are not the best candidates for efficient use of GPUs given their relatively small compute load, the potential role of GPUs for offline regridding weights generation could be considered; this shall be done in a way not to have to rewrite it every two or three years as it may take some time before we can rely on one sustainable programming model

• Support of dynamic process and threads affinity, C4, in ticket #2351

Running an application with proper process and thread affinity, given the specific architecture and memory hierarchy of the computer platform, is crucial for efficiency and performances. 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. A typical example is when component model processes are successively used by the coupling library to calculate regridding weights and then to run the component model per se. The coupler should be able to adapt to this situation. First prototyping tests have been performed with Hippo, a tool that dynamically rebinds processes and threads to match the different phases of the application with calls from within the application code. They have to be continued and generalised.

• Support OpenMP models, C4, in ticket #2361

We know of few users who couple OpenMP models with OASIS3-MCT. An attempt was made in ESiWACE to make OASIS3-MCT evolve to become multithreaded and thread safe in order to fit the calling program multithreaded. Finally, it was considered too complex and only the SCRIP library is now multithreaded. It has been

decided not to aggressively pursue this further inside OASIS3-MCT for now. If the community need arises at one point in the future, we would reconsider this task. Ticket #1223 is closed and this issue is now mentioned in ticket #2361

• Interoperability with other couplers, C3, in ticket #2361

This question of interoperability with other coupling software, in particular with ESMF should be addressed. Potential use cases, e.g. an ESMF coupled system containing an OASIS3-MCT-coupled application, exist in the community. This question would probably be better addressed by groups confronted to a specific use case, by asking for dedicated support. An OASIS developer could visit the group to better understand the technical implications and develop a first prototype. It would then be easier to evaluate the technical implication of a generalisation of this feature.

• Develop standard components for standard workflow tasks, C2, in ticket #2361

This is to develop (or collect existing ones in the community) and distribute "standard" components that would be coupled by OASIS3-MCT to the coupled model for basic tasks in the workflow such as data readers and writers.

Conclusions

This document proposes an update of the OASIS3-MCT development plan, detailing the tasks planned on the short term for the next release, OASIS3-MCT_5.0 due in December 2021, covered by IS-ENES3 and ESiWACE2 funding. The major development is the interfacing with a new regridding library in addition to the SCRIP library for better performance and quality.

In the mid-term, first steps toward dynamic coupling are foreseen. In the longer term, different issues, in particular the ones presented in section 3 above, will have to be addressed to answer the challenges posed by the exascale era. The question of merging with other tools developed in the community such as ATLAS or XIOS will also have to be considered. In all cases, it is evident that no step change in OASIS3-MCT can be envisaged with only the limited funding confirmed today (i.e. 0.5 FTE from CNRS, 0.5 FTE by CERFACS). Additional national or European funding or other collaborative development organisations will have to be identified, in the framework of the ENES sustainability plan being currently discussed in the community.

This development plan discussed and approved by the OASIS Advisory Board.

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