

IS-ENES3 Deliverable D8.2

OASIS3-MCT_5.0 release

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ABSTRACT

The developments realised for the last version of the OASIS coupler, OASIS3-MCT_5.0, are described. This release forms the heart of IS-ENES3 deliverable D8.2. It includes the developments identified in IS-ENES3 DoW and most of the ones listed in Milestone 8.3 “Final list of developments for OASIS3-MCT_5.0”, onto which the latest Development Plan endorsed by the OASIS Advisory Board in November 2020 is based.

The most important tasks are 1) a complete benchmark of SCRIP, ESMF, XIOS and YAC regridding functionality; 2) a unified scripting environment to calculate the regridding weights with SCRIP, ESMF and XIOS; 3) Python and C bindings; 4) a new load balancing analysis tool; 5) diagnostics and field combination; 6) new options for existing coupling transformations.

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Revision table			
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Executive Summary

This document details the developments realised for the last version of the OASIS coupler now available, OASIS3-MCT_5.0. This release forms the heart of IS-ENES3 deliverable D8.2 linked to WP8 Task 3 “OASIS3-MCT development”.

OASIS3-MCT_5.0 includes the developments identified in IS-ENES3 DoW and most of the ones listed in Milestone 8.3 “Final list of developments for OASIS3-MCT_5.0”, onto which the latest Development Plan endorsed by the OASIS Advisory Board in November 2020 is based.

The most important tasks realised are:

- an in-depth analysis of the SCRIP, ESMF, XIOS and YAC regridding functionality including the realisation of a complete benchmark;
- the provision of a unified scripting environment for SCRIP, ESMF and XIOS so that users can test these three libraries and evaluate their quality for selecting the sets of regridding weights to use in their coupled application;
- the provision of python and C bindings allowing full support of coupling with Python and C codes;
- the development of a new load balancing analysis tool, which outputs the full timeline of all coupling related events for all allocated resources of a coupled simulation;
- additional coupling transformations and operations, in particular diagnostics and field combination;
- new options for existing coupling transformations.

Significant resources were devoted to improve the OASIS3-MCT coupler in IS-ENES3. This results in a new version, OASIS3-MCT_5.0, with many new options. Additional future developments are foreseen but most of them depend on the procurement of additional contract resources even if some will be funded by Cefracs internal resources.

1. Objectives

This document details the developments realised for the last version of the OASIS coupler now available, OASIS3-MCT_5.0 [Valcke et al, 2021 b]. As described in IS-ENES3 DoW, this deliverable is linked to WP8 Task 3 “OASIS3-MCT development”.

The developments identified in the DoW for the OASIS3-MCT_5.0 release were the following ones:

- parallel and higher-accuracy library for the calculation of the interpolation weights;
- further development of LUCIA, the load balance analysis tool;
- diagnostics and pre- and post-processing transformations;
- development of Python bindings.

This list was completed in Milestone 8.3 “Final list of developments for OASIS3-MCT_5.0”¹, onto which the latest Development Plan endorsed by the OASIS Advisory Board in November 2020 [Valcke et al 2020] is based. The objective was then to implement these developments in the coupler. All these developments, described in detail in section 2.1, are now included in OASIS3-MCT_5.0², except the following ones that were finally not considered having high priority³:

- Conformance of OASIS3-MCT with CMIP6 standard for weight file format, ticket #[2401](#) : this was discussed in the CMIP6 framework but was finally postponed as the file format itself was not clearly defined.
- Analysis and optimization of the memory use in OASIS3-MCT, ticket #[1104](#): this has been delayed as we had no user feedback about any memory problem.
- Environment to create fractional areas⁴ for truly conservative remapping, ticket #[2460](#) : this environment is currently under development and will most probably be added in the official release in the next month or so.
- Content of debug files for EXPOUT coupling field, ticket #[2365](#) : the demand is to add the field grid in the debug file and, in case of bundle fields, to have all bundles written out to the same debug file; this has been postponed for the next release.

Other developments, not targeted at the time, were included in OASIS3-MCT_5.0, as they rapidly answered specific user needs that emerged in the last year or so. These are described in section 2.2.

We note that almost all these developments were funded by IS-ENES3, except few ones covered by ESiWACE2⁵, which are specifically identified as such below.

Finally, we conclude this document with some perspectives on the future possible evolution of OASIS3-MCT.

¹ https://is.enes.org/documents/milestones/m8-3-final-list-of-developments-for-oasis3-mct_5.0/view

² See <https://oasis.cerfacs.fr/en/downloads/> to get OASIS3-MCT_5.0 sources.

³ For each item, we refer to the related Redmine ticket at <https://inle.cerfacs.fr/projects/oasis3-mct>. If you wish to have access to the Redmine, click on “Register” in the upper right corner; your request will be answered rapidly by Cerafacs administrators.

⁴ To have a coherent ocean-atmosphere coupled model, the best practice is to define fractions of water and land in the atmosphere cells based on the conservative remapping of the ocean sea-land mask.

⁵ <https://www.esiwace.eu>

2. Results: content of OASIS-MCT_5.0 release

2.1 Developments identified in Milestone 8.3

Interpolations & transformations

- Interfacing with a high-quality parallel library for the calculation of the regridding/interpolation weight-and-address file, tickets #[2349](#) & #[1011](#)

This is one of the main tasks funded in IS-ENES3. The objective of this work was to offer other regridding possibilities than the SCRIP library in the OASIS3-MCT coupler. Therefore, we have investigated different software used in Earth System Modelling, i.e. ATLAS, MOAB-Tempest Remap, YAC, ESMF, and XIOS. This study is detailed in [Valcke et al, 2021 a]; see also [Piacentini 2020], [Jonville & Valcke 2019] and [Valcke & Piacentini 2019].

A first preliminary analysis led us to conclude that ATLAS and MOAB-Tempest Remap are certainly appealing libraries but their usage for regridding in OASIS3-MCT cannot be recommended at this point in time.

Then we developed a benchmark environment to evaluate more precisely SCRIP, YAC, ESMF, and XIOS regridding functionality; five regridding algorithms were evaluated for four different functions for seven pairs of grids used in real ocean or atmosphere models. The benchmark conclusion was that YAC, ESMF and XIOS can all be considered as high-quality regridding libraries, while some details still need to be fixed. We also proceeded to a very first performance analysis of SCRIP, ESMF and XIOS which shows that both ESMF and XIOS show much better ($O(100)$) performance than the SCRIP.

At that point, instead of choosing one new library among the ones that we evaluated and replacing the SCRIP with it, we decided to keep the horizon more open, in agreement with our users. We think that it will be more beneficial to help our users to test and use those different libraries so that they get more experience and so that we get their feedback before investing more effort into interfacing one particular library into OASIS3-MCT. We therefore provide with OASIS3-MCT_5.0 sources, a unified scripting environment (see directory `oasis3-mct/examples/regrid_environment` and documentation therein) for SCRIP, ESMF and XIOS so that users can test these three libraries on their own grids and evaluate their quality before selecting the sets of regridding weights to use in their coupled application. However, as some of our users will most probably keep on using the SCRIP library for some time, we still brought some (non-major) improvements to this library, although not investing a lot of manpower in this library anymore.

- Conservative remapping for the runoffs, 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 should receive a value but it is necessary that all source grid points find a target on the ocean grid. The method proposed by Aurore Volodire at CNRM, based on the regular interpolation weights but taking the reverse interpolation links, is implemented in OASIS3-MCT_5.0. This method

allows to conserve the river outflow locally and globally. Details are available in [Maisonnavé 2020] and in section 4.3 of the User Guide (see LOCCUNIF, LOCCDIST and LOCCGAUS).

- Improved and additional diagnostics, tickets #[2356](#), #[1761](#) and #[1069](#)

Diagnostics performed under the CHECKIN/CHECKOUT operations were revised. These operations now calculate the global minimum, maximum, mean, and sum of the source/target field values taking the mask into consideration. If a grid area or fraction field is also available, the area and/or fraction weighted mean and sum are also diagnosed and written out to the output file. See the User Guide, sections 4.2 and 4.3.

- (Pre- and) post-processing transformations, ticket #[2364](#)

Post-processing operations under BLASNEW, which performs a scalar multiply or scalar addition to any destination field, were extended. In addition, other fields on the destination side can be added with a multiplier and addition weight. We limited the developments to this relatively simple possibility only as we consider that in most cases, specific post-processing transformations (like combination of the coupling field with observations) can be easily much more coded in the models themselves⁶. See the User Guide, section 4.4.

- Normalisation by the grid cell “true” area for the conservative remapping, ticket #[1010](#)

The approximations adopted by the SCRIP library impact its estimation of the grid cell areas. Therefore, to have an exact conservation of the field surface-integrated values, a correction based on the ‘True’ (TR) area of the cells can be applied by choosing DESTARTR, DESTNNTR, FRACARTR or FRACNNTR options. These are based respectively on DESTAREA, DESTNNEI, FRACAREA and FRACNNEI normalisations adding the so-called “TR correction”: the true area of the cells, i.e. the ones considered by the component model itself, are used in the remapping normalisation. See the User Guide section 4.3.

- Number of neighbours used in the regridding weight file name, ticket #[2350](#)

The number of neighbours used in the regridding is now included in weight file name so to avoid confusion when the same interpolation is used between the same grids but with different number of neighbours for DISTWGT, DISTWGTNF, GAUSWGT, GAUSWGTNF LOCCUNIF, LOCCDIST or LOCCGAUS regriddings.

- Easy detection of the target grid point that do not receive any value, ticket #[731](#)

This is not supported directly by OASIS3-MCT itself but can be realised by using the regrid_environment environment (see the User Guide section 6.3.3): the received field is transformed to give the value of 10000 to masked target points and the value of 1.e20 to non-masked points that do not receive any interpolated value (if any), in order to be able to easily detect them.

- Specification of Lambert projection north thresh and south thresh values in the *namcouple* configuration file, ticket #[2459](#)

⁶ We also think that user needs with respect to this functionality are low, as nobody answered the mail and reminder that was sent on the OASIS user mailing list about their corresponding requirements.

\$NTHRESH and \$STHRESH can now be specified in the *namcouple* configuration file. These are the values of respectively the northern and southern latitude (in radians) above and below which the hypothesis about the cell boundary definition for the area computation in SCRIPR/CONSERV switches from linear boundaries in longitude and latitude to a Lambert equivalent azimuthal projection.

Communication

- Extension of the `oasis_get_intracomm` API (Application Programming Interface) routine to support multiple components, ticket #[2687](#) (this development was officially funded under ESiWACE2)

The API routine `oasis_get_intracomm` merges two MPI communicators from two different components to form a new communicator. This routine was extended in the new `oasis_get_multi_intracomm` API routine to support more than 2 components. A list of component names is now passed as an array argument. This is needed in coupled models involving both OASIS3-MCT and XIOS when XIOS manages the output of ensemble simulations. See the User Guide section 2.2.9.

- Sending/receiving simple scalars, ticket #[1937](#)

Coupling scalar variables is possible using OASIS3-MCT_5.0 available API. Scalar variables are variables such as date and time, logical flags, integer or real parameters, or other scalar data that might be defined identically across all MPI tasks in a component or even just on a subset of tasks. The procedure to implement this type of exchange is described in detail in the User Guide, section 2.5.2.

Other functionalities

- Further development of LUCIA, the load balance analysis tool, tickets #[2357](#) & #[1003](#)

LUCIA was the tool delivered with OASIS3-MCT to automatically evaluate the load balance of the coupled components. This tool was completely revised in collaboration with the Barcelona Supercomputing Center (BSC) and a new load balancing analysis tool is now available. It can be simply activated through the *namcouple*. When activated, this functionality outputs the full timeline of all OASIS3-MCT related events, for all allocated resources. This timeline is saved in one NetCDF file per coupled component. It provides the comprehensive sequence of all operations related to the coupling (field send and receive through MPI, field output on disk, field interpolation and mapping, field reading on disk, restart writing, initialisation and termination phase of the OASIS3-MCT setup) so that any simulation slowdown in link with the use of the OASIS3-MCT library can be identified. See the User Guide, section 6.5, [Maisonnave et al 2020] and [Piacentini & Maisonnave 2020].

- Python bindings, ticket #[2362](#) and #[2509](#)

OASIS3-MCT_5.0 comes with full support of python and C bindings. First, the OASIS3-MCT Fortran code is wrapped in Fortran using ISO-C bindings, which are subsequently wrapped in C. Finally, the C is wrapped in Python. The python wrapper functions and the Fortran-python API correspondence are fully described in the User Guide section 2.4. Equivalent Fortran, python and

C examples are provided. Python bindings will bring OASIS3-MCT to a much wider ecosystem and is a good way to attract countries less advanced in HPC. This required an update of the compiling environment, see next item below. For details, see [Gambron et al, 2021].

- Update of compiling environment, ticket #[2509](#) and #[2689](#) (this development was officially funded under ESiWACE2)

We took the opportunity of the support of Python bindings to update the compiling environment. In particular, we interacted with MCT developers to support gnu10 compiler with MCT, and therefore updated to MCT 2.11 version. We also updated all header Makefiles in directory util/make_dir.

- Develop, maintain, and systematically apply the buildbot test suite, ticket #[232](#)

Buildbot is a software used to recompile automatically the OASIS3-MCT sources when a development is committed on the Git master version of the sources or on an active Git branch and then to perform tests with toy models to see if the development did not introduce any bug in the sources. To do so the results are compared automatically to the results of a reference state that was verified. The use of Buildbot allows to detect some problems and solve them before other developments are done.

The old Buildbot test suite used toys testing multiple functionalities and toys from users. A new Buildbot tests suite was constructed in 2019-2020 based on the functional toy concept. Each of the ~30 toys included now tests one functionality of the OASIS3-MCT coupler. See [Coquart et al, 2021].

- Updated API interface for `oasis_def_var`, ticket #[2273](#)

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. See the User Guide, section 2.2.5

- Systematic tests of NetCDF returned error code, ticket #[550](#)

Systematic check of error code was implemented for all NetCDF calls in OASIS3-MCT_5.0.

Support and training

During the whole IS-ENES3 period, we have been delivering high quality user support through the forum, by mail or by phone, and we will keep on doing so until the end of the project. We also delivered one face-to-face training to 3 persons in May 2019 and we have developed a SPOC (Small Private Online Course) on “Code Coupling with OASIS3-MCT” thanks to ESiWACE2 funding. Two SPOC sessions have already been organized, one in July 2020 with 10 participants and one in May 2021 with 11 participants. Also, 5 PMs of Dedicated User Support has been provided within IS-ENES3 and there are still 4 PMs to be delivered in ESiWACE2 in 2022 and 3 PMs in IS-ENES3.

- Toy coupled models, tickets #[2555](#) and #[2175](#)

Practical examples, in the form of toy coupled models, are also delivered with the OASIS3-MCT_5.0 sources, to help users to learn about the coupler. These are available in OASIS3-

MCT_5.0 `oasis3-mct/examples` directory. They are described in section 6.3 of the User Guide.

- Toy ATM-NEMO for OASIS3-MCT users, ticket #[2402](#)

An atmosphere toy, TOYATM, that can be coupled to the real ocean code NEMO was developed and is distributed with the sources of NEMO. See details at https://forge.ipsl.jussieu.fr/nemo/wiki/2020WP/VALID-11_clevy_OASIS_TESTCASE.

- Migration from SVN to GIT for source management, ticket #[2352](#)

OASIS3-MCT source management was migrated from SVN to GIT in November 2019. 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.

- Migration of the OASIS3-MCT web site from DKRZ to Cefracs, ticket #[2697](#)

The OASIS3-MCT web site is now hosted at Cefracs using the content manager Wordpress, see <https://oasis.cerfacs.fr/en>. The old site at DKRZ, using Plone, is no longer valid.

2.2 Additional developments

As stated in Section 1, some developments were not planned in Milestone 8.3 but were realised to answer specific user needs or to solve bugs that popped up during the course of the project.

- Support for different NetCDF file formats ticket #[2730](#) (this development was officially funded under ESiWACE2)

A new optional keyword `$NCDFTYP` is now available in the `namcouple` to indicate the NetCDF file type for all (i.e. mapping, restart, output) new NetCDF files generated by OASIS3-MCT_5.0. The options are `cdf1`, `cdf2` and `cdf5`. The mode `cdf1` is also known as classic mode, `cdf2` as large file format or 64bit offset and supports larger files, `cdf5` as 64bit data and supports both larger files and larger variables.

- Support of regridding without the nearest-neighbour fill, ticket #[731](#)

By default, `DISTWGT`, `GAUSWGT`, `BILINEAR`, and `BICUBIC` operations provide values for all non-masked target grid points, using the non-masked source nearest neighbour value for non-masked target points that did not receive a value with the original algorithm (if any). New options `DISTWGTNF`, `GAUSWGTNF`, `BILINEARNF`, and `BICUBICNF` do not activate this filling which means that some non-masked target grid point may end up with no regridded value.

- Options `GSSPOS` and `BSSPOS` for global `CONSERV`, ticket #[2327](#) (this development was officially funded under ESiWACE2)

Different options are available for the global conservation operation `CONSERV`. With `GLBPOS`, the field is integrated on the non-masked cells of the source and target grids, and the residual (target - source) is distributed proportionally to the value of the original field as a multiplicative term. With the new option `GSSPOS`, the same is done except that the multiplicative term is computed

separately for positive and negative values of the field. This ensures the global conservation of the field and, as GLBPOS, does not change the sign of the field. It should be used in cases where the area averaged field value tends to 0 as these cases can generate poor corrections, even leading to changes of sign, when carried out with the GLBPOS option.

With the other new option BSSPOS, an analogous procedure is applied except that the non-masked surface of the source and the target grids are taken into account in the calculation of the residual. This does not ensure global conservation of the field but ensures that the energy received is proportional to the non-masked surface of the target grid and it does not change the sign of the field. A detailed study of the impact of the different options can be found in [Craig 2019].

- Bugfixes included in OASIS3-MCT_5.0 are listed here; more detail can be found in the tickets mentioned:
 - Abort with NOINTERP when only a subdomain of the global grid is coupled, which turned out to be a problem with NEMO; an update of NEMO sources with a version more recent than 4.0.3 solves this problem, ticket #[2472](#)
 - Problem with SCRIPR/BILINEAR periodicity, ticket #[2419](#)
 - SCRIPR/GAUSWGT: exact calculation of average distance between two source grid points, ticket #[2399](#)
 - Calculation of local distance in SCRIPR/GAUSWGT interpolation [Maisonnave 2019], ticket #[2500](#)
 - SCRIPR/BICUBIC and BILINEAR sequence in weights generation”, ticket #[2725](#)
 - Component name argument in `oasis_get_intercomm`”, ticket #[2776](#)
 - Update `oasis_abort` with writing to unit 0, ticket #[2678](#)
 - Problem with array bounds check for `cplfind`, ticket #[2655](#)
 - Fix error in `maxloops/kfac` computation in `oasis_mpi_reducelists`, ticket #[2654](#)
 - Load balancing tool compatibility with CRAY compiler, ticket #[2473](#)
 - Problem in `m_MCTWorld.F90` in the routine `initm`, ticket #[1321](#)

3. Perspectives and conclusions

Some significant resources were devoted to improve the OASIS3-MCT coupler in IS-ENES3. The developments realised followed closely the Development Plan approved by the Advisory Board in November 2021. These developments, described in this report, are all included in the new OASIS3-MCT_5.0 version.

One important decision we took concerns the regridding library. Instead of choosing one new library among the ones that we evaluated and replacing the SCRIP library with it, it was decided to provide a unified scripting environment allowing to use either SCRIP, ESMF or XIOS to calculate the regridding weights. This allows users to test these three libraries on their own grids and evaluate their quality before selecting the set of regridding weights to use in their coupled application. The drawback of this approach is that users have to install ESMF and XIOS themselves on their platform, which is not necessarily easy. One possibility to facilitate the use of this unified

scripting environment would be to deliver the whole environment using a container technology such as Docker or Sarus. This will be considered for a future version of the coupler.

The other evolution that would imply choosing one regridding library, or different parts of the different libraries, and interfacing it or them directly in OASIS3-MCT is the support of dynamic grids, which are grids with grid points and cells evolving during the simulation. This implies that the calculation of regridding weights necessarily has to be redone dynamically on-line during the run. The full support of dynamic grids is however not planned in the short term and therefore the calculation of regridding weights prior to the run or during the initialisation phase, as currently supported, should fit user needs for still few years.

However, an evolution that we consider on the short and mid-term is the support of components with grids having a mask evolving with time. Indeed, examples of coupled systems including dynamic masks already exist, e.g. ice sheet or sea ice models. As a first step, dynamic masking via weighted mapping capability (i.e. with no new weights generation per se) will be considered. The current weight generation implementation, either before the run or in the initialisation phase, will therefore still be valid for that extra step of support of grids with dynamic masks.

Regarding the regridding libraries evaluated in [Valcke et al, 2021 a], we also note that our evaluation included a first performance analysis of those libraries that could certainly be pushed further. We evaluated the scalability curve for the 1st O conservative remapping from the NEMO ORCA12 t12e source grid to the high-resolution icosahedral grid on Cerafacs cluster kraken (Intel Skylake nodes) for up to about 1000 cores for SCRIP, ESMF and XIOS. We could certainly evaluate the scalability of the regridding weight calculation on other platforms for higher number of cores for other algorithms and other grids to produce a more complete performance analysis.

Another issue that we have to address, given the evolution of the computing platforms, relates to the behaviour of the coupler on heterogenous hardware, e.g. CPU-GPU systems. Although couplers are not the best candidates for efficient use of GPUs given their relatively small compute load, the potential role of GPUs for regridding weights generation should be considered. We should also test the coupling with OASIS3-MCT between two components, one running on GPU and another one on CPU. Such coupled implementation has already been tested at Cerafacs for CFD codes with CWIPI, another coupling library also based on MPI. In principle it should work with OASIS3-MCT but this still has to be tested.

To be complete, we mention here that in addition to the developments that we already mentioned in section 1 (i.e. the conformance of OASIS3-MCT with CMIP6 standard for weight file format, the analysis and optimization of the memory use, the environment to create fractional areas for truly conservative remapping, the content of debug files for EXPOUT coupling field), we should also consider on the longer term the support of vertical interpolation and the modernisation and extension of *namcouple* syntax.

Further developments may be funded by Cerafacs internal resources but most of them are dependent on the procurement of additional contract resources.

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