Biogeochemistry coarsening in NEMO 4.2

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Abstract

This work aims to support UKESM to adopt a degraded resolution coupling, based on the OASIS based solution previously implemented in NEMO-PISCES, but using the MEDUSA BGC model instead. Both of these component models will ultimately also need to be coupled separately to the UKESM atmosphere (based on the Unified Model). The first preliminary task achieved here deals with the upgrade of the NEMO coarsened code from 3.6 to 4.2 version. The second task merges the Mercator Ocean development based on AGRIF that allows to produced, in a simplified way, the coarsened bathymetry input files. A one month long simulation coupling an ORCA025 ocean and an ORCA075 TOP-PISCES BGC validates at first order our interfaces and coarsening algorithm. This updated and simplified version of our OASIS based coarsened BGC model is made available in the NEMO GitLab to prepare the future PISCES-MEDUSA switch.

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This document describes the next step towards the implementation of an ocean with biogeochemistry (BGC) model at hybrid resolution. The preliminary steps consisted in the splitting of the two NEMO [1] components into two separated executables [2], coupled via the OASIS library [3] and adapting interfaces and coupling library to a coarsening algorithm [4] in such a way that it was possible to reduce the BGC resolution from the ocean ORCA025 grid to 1/3 [5]. This work aims to support UKESM to adopt the same degraded resolution coupling, but using the MEDUSA BGC model instead of the PISCES release component.

Furthermore, while the specificity of this request is to support coupling between degraded resolution NEMO fields and MEDUSA, both of these component models will ultimately also need to be coupled separately to the UKESM atmosphere (based on the Unified Model). This likely has implications for the sequencing of events in the coupling between NEMO and MEDUSA and NEMO/MEDUSA and the Unified Model, leading to deal with three different model grids and associated land-sea masks.

UKESM is the main UK Earth system model. UKESM models are used for scientific research and to provide policy guidance, both direct to the UK government and indirectly through assessments such as the recent IPCC AR6 report. A new version of the model, UKESM2, is under development and intended for use in a future CMIP7 exercise, and possibly increase the ocean resolution in UKESM2 from 1° to 0.25°. To do this, while retaining the necessary computational throughput, it is necessary to find ways to make the BGC model, MEDUSA, run faster. One option for this is the dynamical field coarsening approach, which would allow to run the BGC model at a 1/3 of the resolution of the dynamical model. Such a development will allow to run UKESM2 with an increased ocean (dynamical) resolution with improvements to many ocean dynamical fields anticipated. These improvements are also expected to feed through to improve the resulting BGC and overall simulation of the global carbon cycle. We hope these improvements lead to more robust estimates of allowable carbon budgets commensurate with staying below certain warming levels, such as the 2°C level set out in the 2015 Paris Climate Agreement.

Before replacing the existing PISCES BGC module by MEDUSA, two preliminary tasks were necessary. Due to their complexity, these tasks represent most of the work described in this document. The BGC model switch and coupling with the UKESM other components will be described in a future report.

The first preliminary task deals with the obsolescence of the current ocean-BGC hybrid resolution model. An upgrade of the NEMO code is necessary, from 3.6 to 4.2 version. This operation is not a simple replacement of the coupling related subroutines, because a new management of row and column duplicated line for periodical conditions. This leads to a new definition of the input and output files, which affects the way the coarsened variables defining the grid are defined.

In addition, we found reasonable to join the efforts of the Mercator Ocean team (Jérôme Chanut & Clément Bricaud) who also aim to develop a coarsened configuration of the BGC model in NEMO, but with a different strategy (the definition of the ocean grid as an AGRIF zoom of the BGC grid). Both AGRIF and OASIS based versions are implemented in parallel, which allows to share, thus accelerate, some developments. In particular, thanks to this collaboration, the pre-processing phase will be strongly simplified, allowing to produce the same input configuration file for both AGRIF and OASIS configurations.

Coarsening algorithm

As previously defined, the T,U,V,F coarsened land-sea masks are deduced from the corresponding fine ocean grids, as shown below:

Grid type	i-index of associated source	j-index of associated source
T	1 to CF	1 to CF
U	CF	1 to CF
V	1 to CF	CF
F	CF	CF

Table 1: indexes in I and j dimension of the grid points involved in the coarsening operations, among all the CF times CF source grid points possibly associated, depending on the NEMO grid type

This clearly differs from the standard strategy that derives the U,V,F grids from the T grids. And this has a consequence on the dimensions of the coarsened grid, deduced from the fine ocean grid and its periodicity.

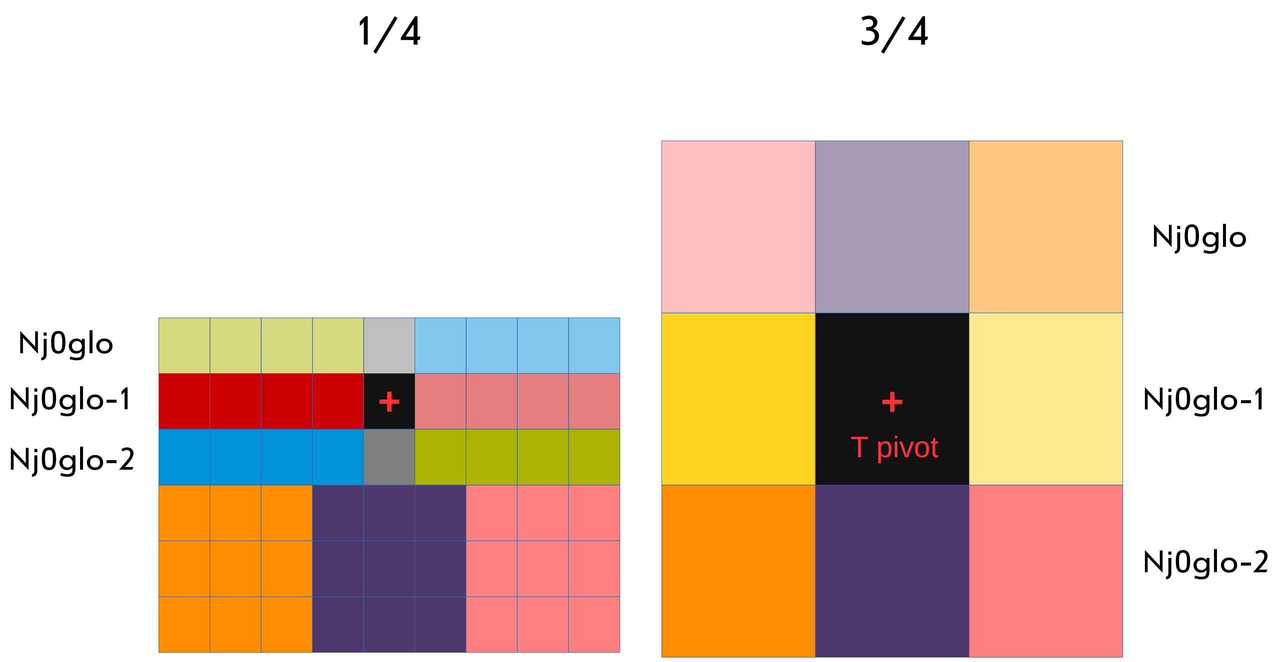

Figure 1: Coarsening of ORCA025 grid points onto an ORCA075 grid (x3), zoom on the North pole folding pivot (T grid). Duplicated grid points are coloured with transparency

For each grid, the total number of line and column must be chosen in such a way that n^2 source grid points would be available for each coarsened target grid point (with n = coarsening factor). To do so, one can include duplicated points in the total number of available source line or column, but has to be careful not to use them twice for conservation reasons. These constrains lead to the 3 cases shown on Figures 1 and 2. This forbids to chose an even coefficient for T pivot grids (`jperio=4`) and leads to transform an F pivot source grid (`jperio=6`) into a T pivot target grid, if an even coefficient is chosen to transform an F pivot grid. The same coarsening algorithm is used for each T,U,V,F grid type.

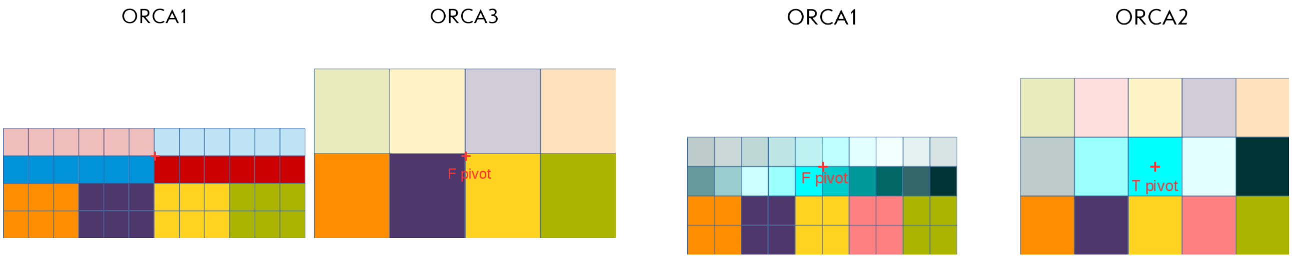

Figure 2: Same than Fig 1, but for ORCA1 (F grid pivot) and odd coarsening coefficient (left), or even coarsening coefficient (right)

Pre-processing workflow

Upgrade of the DOMAINcfg configuration file tool

In our previous pre-processing workflow, several manual operations were necessary to produce the configuration file of our coarsened grid. Recent developments in AGRIF have made possible the definition of AGRIF zooms matching exactly the geographical boundaries of the mother grid. Thanks to this improvement, AGRIF can be use for coarsening. The coarsening algorithm described in the previous § was added to the AGRIF library, making possible, by linking the library with the `DOMAINCfg` tool, the production of the source ocean grid and the target coarsened grid at the same time. The compiling must be done after a CPP pre-processing (`key_agrif`). The new tool sources have been made available in a `dev_agrif_coarsening` branch of the NEMO GitLab by the Mercator Ocean team. We exactly copy this development in a second `dev_oasis_coarsening` branch, that will also include the modifications made in the NEMO code to include the OASIS coarsening interfaces.

For validation of this new `DOMAINCfg` tool, the same input files are used with the old workflow (same coarsening algorithm) and the resulting configuration files compared. No differences are noticed, which leads to replace our previous workflow by this single and easier-to-use tool.

As already noticed, this algorithm can produce slightly unrealistic coarse bathymetry. In particular, isthmus can be opened and straights closed. In addition, the way U,V & F bathymetries are produced (derived from the fine U,V, & F grids instead of from the coarse T grid) could lead to inconsistencies in the tracer advection scheme. These problems will be investigated when it will be possible to compare long term full resolution and mixed resolution simulations. Notice that our bathymetry generation mode still allows to adjust the land/sea mask after this pre-processing generation phase (by-hand modification of the coarse `DOMAINCfg` file).

Upgrade of the OASIS weights generation tool

However, the AGRIF procedure does not produce the OASIS weight & address (W&A) files that allows to coarsen the model variable at runtime. Said differently, the coarsening algorithm, included in the AGRIF library, was used by `DOMAINCfg` to coarsened the input variables such as the 3D land sea mask or fixed horizontal scale factors, but this algorithm is still needed at runtime to coarsen the time dependent ocean variables, which is done, in this work, via OASIS.

Consequently, it is necessary to refurbish the existing tool that creates these W&A files[1]. In this new version, the two source and target land-sea masks are read from their corresponding `meshmask` files (produced in a first step by the `DOMAINcfg` tool, in addition to the configuration files). The coherence of the two grids is checked (pivot type, dimensions), the coarsening algorithm applied to associate n^2 (or less if masked) source grid points to every non masked target grid point. Notice that our algorithm does not detect the possible source grid points left unused.

These new development greatly simplify the pre-processing workflow and facilitates the set up in our implementation work. It is saved to the `dev_oasis_coarsening` branch.

Upgrade of the NEMO coupling interface

Since the OASIS interfaces in both ocean and BGC (OFFLINE model) are not intrusive in the source code, it becomes quite simple to re-implement them at every version change. These developments are also saved to the `dev_oasis_coarsening` branch[2]. The input file dimension change, introduced by the 4.2 version, does not affect the partitioning description communicated to OASIS. A simple coupling, without coarsening and relying on the ORCA2 grid is quickly set up. Despite problem with the mixed layer, that must be recomputed in the BGC interface or bounded near the north pole folding, a one month long simulation was produced. In a future step, it will be necessary to check the similarity of both coupled and uncoupled results.

1 Located in the NEMO directory `tools/CRS_WEIGHTS`

2 named `85-bgc-coarsening-with-oasis` on NEMO Gitlab `https://forge.nemo-ocean.eu/nemo/nemo.git`

Validation

The same validation simulation is performed with the target ocean (ORCA025) – BGC (ORCA075) configuration. Input files were produced on both resolution. Both ORCA2-ORCA2 (no coarsening) and ORCA025-ORCA075 (coarsening) simulations were performed with the same executables.

We compare the results of two one month long simulations lead with the ORCA025-ORCA075 configuration in one hand and with the ORCA025 full resolution mono-executable on the other hand. No major differences are noticeable, which validate our interfaces and coarsening algorithms at first order.

Computing performances are close to the one already measured with the 3.6 model, even though NEMO computation speed up stresses the important contribution of the 3D OASIS coupling to the total simulation time. As can be seen in Fig. 3, the time spent to coarsen and communicate the ocean variables to the BGC model remains unchanged.

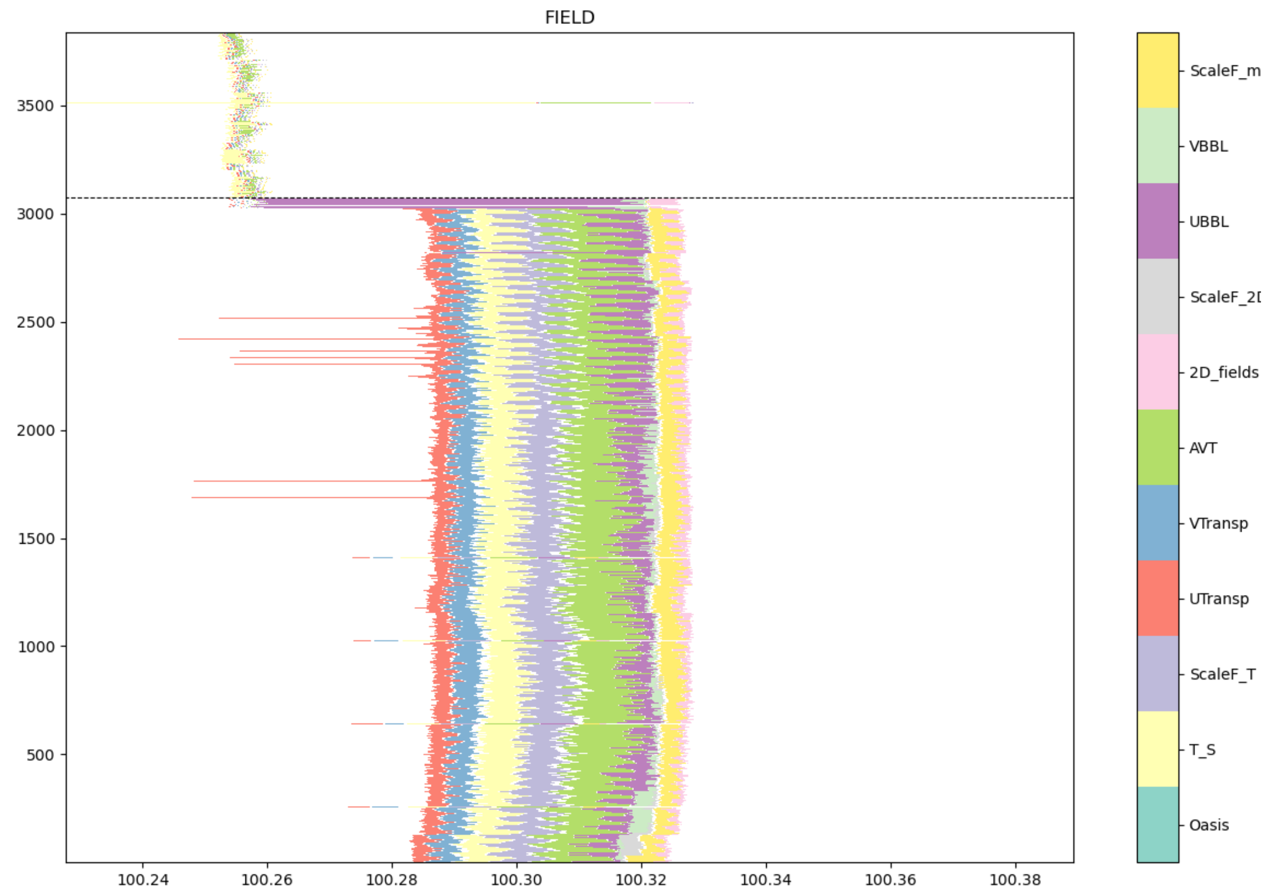

Figure 3: Coupling event timeline, displayed for 0.2 second elapsed time (x-axis) of a sequential one way coupling ocean_ORCA025-BGC_ORCA075 coarsened simulation performed on 3072 (ocean, lower part of the plot) and 384 (BGC, upper part of the plot) cores (y-axis). Each colour stands for one group of coupling field (sent and interpolated by the ocean, received by the BGC component)

Next steps

Our upgraded ocean-BGC interface with coarsening is able to provide coherent ocean variables to the BGC model. But this does not mean that the major requirement that justifies to implement a coarsening algorithm in place of a standard interpolation, the conservation of the ocean quantities, is fulfilled.

In that perspective, several complementary actions are required. Conservation is hard to achieve close to the land-sea mask boundaries (bathymetry), if the source grid point number associated to the target grid point falls below the standard value of n^2. In the horizontal plan, the coarsened mesh surface seems to introduce a distortion, that can be avoided in the open ocean areas by using the multiplication of the coarsened scale factors (`e1x`/`e2x`) instead. At the opposite, in the vertical direction, to avoid numerical overflow, one would have to select the BGC equations that would preferentially use, close to the bathymetry, the maximum of source `e3x` scale factor instead of its (average) coarsened value.

From the numerical performance point of view, it would be interesting to try to reduce the accuracy (single precision) or the number of 3D scale factors exchanges, thus to limit the coupling overcost. In particular, a computation of these target grid scale factors from the coarsened sea surface height could be investigated (`qco` option). Of course, this will have to be done with conservation requirements in mind.

In the same perspective, a decrease of the coupling time step equal to the current online BGC model calling frequency would reduce both BGC and coupling overcost by at least a factor `n`. In this configuration, average values would have to be transmitted to the BGC model, except for the scale factors involving the vertical dimension.

In parallel, the PISCES/MEDUSA BGC model switch would have to be initiated, first by replacing the BGC subroutine call in the single executable configuration, then the offline BGC model, to finally allow to plug the MEDUSA OFFLINE configuration to our coupled ocean module.

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