NEMO Development Strategy 2023-2027

Version 1.0 11th November 2021

NEMO Developers Committee

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1 Introduction

This first draft of the NEMO Development Strategy (NDS) for 2023 – 2027 is the natural successor to the NDS 2022-2026. Its chapters have been designed to:

a) Capture the main areas where development of NEMO will be important
b) Organise the work into working groups of people who can work efficiently together and make proposals for funding of their area
c) Align with the existing working groups unless there are good reasons to change
d) Make it clear who will lead on each topic
e) Either avoid or clearly identify difficult overlaps between working groups

The order of the chapters is not so important, but has been chosen to give a natural flow from one chapter to the next.

Chapter 2 aims to capture the drivers and requirements for NEMO development expressed by the consortium members. It builds on the experience gained from the corresponding chapter of the previous NDS but it needs consolidation as some members (CNRS and the Met Office) were unable to consult fully internally before the deadline for this draft. The views of members are likely to be consolidated into a single view in the final document; at this stage the responses to most questions have simply been collated. It is intended that there will be some iteration between WGLs and the consortium representatives over the coming six months to ensure that the priorities identified in the final strategy take account of both the technical opportunities and the drivers and requirements.

For this draft, the lead authors of each chapter have been asked to identify the main issues they intend to address in the final document. In some cases, the lead authors have been appointed only relatively recently (e.g. the eddy parametrisation, tools and community support chapters) so the chapters do not go beyond that. In other cases (e.g. the sea-ice and land-ice chapters) the text is fairly well developed. Most chapters are at an intermediate stage of development.

2 Drivers & Requirements for NEMO

2.1 Priorities of Consortium members

Q1. DRIVERS FOR EVOLUTION

1a) What are the target applications for NEMO in your institution by 2026?

- Cover short-term predictions to climate simulations (CMCC, Met Office)
- Ensemble forecasting systems (CMCC, Mercator, Met O)
- Very high resolution (1/36^{o}) global systems, 10-30 day predictions (CMCC, Mercator)
- Global at a hierarchy of resolutions: 1, ¼ and 1/12 some including tides and other aspects of shelf-seas physics (NOC, Met Office)
- Regional simulations from 1/12o down to 1 km or higher (CMCC, Mercator, Met Office, NOC)
- Simulations include BGC (CMCC, Mercator)
- Simulations are often part of Earth System models (CMCC(?), Met Office, NOC(?))

1b) What should be the key drivers for NEMO evolution by 2026 and beyond ?

Specific issues with dynamics / physics

- Sub-grid-scale parametrisation (NOC, Met Office)
- Tidal simulation (Mercator, NOC)
- More flexible vertical coordinate system (Met Office)

Physical interfaces

- Improved coupling between A, W, I, O, BGC (CMCC)
- Improved interfaces with hydrological/coastal/estuarine models (CMCC, Mercator, NOC)

Computational efficiency, nesting and coarsening

- Adaptation to emerging HPC architectures and data handling (CMCC, NOC, Mercator, Met Office)
- Downscaling (CMCC, Mercator, Met O)
- Effective approach to grid coarsening for BGC (NOC)

Verification and validation

- Robustness and reproduceability (Mercator)
- New opportunities for improved code management and verification (Met Office)
- Improved validation using observations (CMCC)

Exploitation of Machine Learning (CMCC, Met Office)

Specific aspects of overall simulations

- Improved simulations of upper layers (Mercator, Met Office)
- Improve ORCA025 Southern Ocean simulation (Met Office)

Possible longer term issues:

- Tighter interaction with atmospheric dynamical cores (eg MPAS) (NOC)
- possible requirement for regional systems at high latitudes (Arctic and Antarctic), including sufficient skill in ice prediction to enable forecasts for navigation purposes (Met Office)

1c) Do you expect to use NEMO for applications close to the coast or up estuaries in the future?

Improving representation of land-ocean interface using estuarine box model coupled to NEMO (CMCC)

Our global systems are aimed to provide tailored/adapted boundaries conditions for coastal systems. We expect that improved land-ocean exchanges could be beneficial even in that context to ensure a better agreement with embedded models. The use of NEMO should then go towards up to littoral zones but not at the estuaries scales. The use of AGRIF to locally refine up to 1km resolution is foreseen (Mercator)

The aspiration for Met Office marine models should be to provide reliable predictions to within 1km of the shoreline and to 5m water depth (chart datum); in practise this requires resolutions of order 250-500m and shallow water physics/numerics including wetting and drying. Met Office already uses a barotropic version of NEMO for storm surge prediction, which implies comparison of SSH data against coastal and estuarine tide gauges. Generic predictions within estuaries are not currently a priority. (Met Office)

Yes, this is a key application for NOC. We note NEMO lacks some capability of bespoke estuarine models – e.g. advection of turbulent properties as the tidal excursion is resolved. This is technically awkward (advection of variables on W grid) so many not be worth it, but remains a limitation in this field. (NOC)

Q2: OCEAN PROCESSES

2a. Which physical processes do you think most need to be improved in NEMO in the future ?

Air-sea interactions parameterization fit for high resolution forcing (including coupling) with available and new parameterizations; vertical dynamics and mixing processes; internal tides; exchanges with rivers to improve boundary conditions; improving lateral open boundary condition schemes (e.g., spectral nudging): understanding overflow and densification processes. (CMCC)

Processes dealing with the OBL boundary layer. This includes bulk formulae, the Atmospheric Boundary Layer (ABL), the interplay between waves and vertical mixing (ex: Langmuir turbulence). (Mercator)

The representation of unresolved or partially resolved mesoscale motions is clearly a rapidly evolving area where NEMO needs to keep up with developments elsewhere (and has a recently formed WG with expertise/experience in these parametrisations). Representation of the upwelling region in the eastern equatorial Pacific is very important but depends heavily on the nn_etau parametrisation. This is unsatisfactory. (Met Office)

The vertical MOC structure. This is too shallow (not specific to NEMO but many (all?) z-level models and also in HYCOM), and goes hand in hand with biases in water mass properties. Most likely there are multiple causes for this (mixing, overflows, air-sea exchanges). Deep water formation (overflows and open ocean convection) is still a major issue. Numerical mixing still seems quite large, so leading to water mass preservation issues. Coastal freshwater input (e.g. through estuarine mixing models) (NOC)

2b. What are the highest priority systematic biases in your target applications?

Improve the vertical dynamics and mixing to achieve a better representation of the thermocline

It still remains a lot of uncertainties in the air/sea; ice/sea interactions and their propagations inside the ocean. Also a better control of systematic error of the input forcing files (systematic bias for example). (Mercator)

The biases in the Southern Ocean in ORCA025 are high priority. Particularly the weak ACC; the fresh bias on Antarctic Weddell Sea coast; the over-active Weddell (and Ross) gyres. The path of Gulf Stream (its separation and the path of its extension off Grand Banks and further east) are still issues. Biases in dense overflows are still issues. There are other biases but they are less easy to characterise (or attribute to particular processes). Mixed layer depths (e.g. the Labrador Sea winter MLD is too deep). Accurate simulation of the eastern equatorial Pacific may well be important because of that region's influence on effective climate sensitivity. (Met Office)

MOC depth, deep water formation and preservation and coastal salinity biases (NOC)

2c. In particular, which processes are critical for each of your target applications as described in Q1

Tidal excursion, coastal upwelling, ROFI dynamics, internal waves/tides, mixing (CMCC)

Air/sea exchanges; Flow-topography interactions; Overflow processes; Tidal motions (Mercator)

The most important processes depend on the time-space scales. For climate simulations: large-scale biases, conservation, model drift, deep ocean spin-up, ice sheet interaction. For the monthly-to-decadal forecasts: representation of natural oscillations like ENSO/AMV/SAM/NAO/PDO/etc., ensemble spread. For short-range predictions: representation of eddies, tides, surface currents and the surface mixing layer. (Met Office)

A realistic ocean mesoscale activity and strength of air-sea interactions. (NOC)

2d. Do you see generalised vertical coordinates as a priority and if so why (less diapycnal mixing or better flow down bathymetry or along bathymetry)?

Both global and regional configurations might benefit from a new generalised coordinate system, e.g. benefits on overflow dynamics, circulation near the sea bed, sinking /cascade, spurious mixing, etc. (CMCC)

Yes. Moving to internal wave explicit modelling will certainly enhance diapycnal mixing. There may be an interest for generalized coordinates to improve biogeochemical fields. (Mercator)

We would like to have greater flexibility for all three of these reasons. An important issue might be to decide whether we want to retain the current form of vertical coordinates as one option and develop a more generalised form as a separate choice. (Met Office)

Yes – all of above reasons and improved benthic boundary layer representation. (NOC)

2e. Do the hydrostatic and Boussinesq approximations need to be reconsidered for some of your foreseen applications ?

Not for our applications. (CMCC)

Relaxing the Boussinesq approximation would ensure a better consistency of the model with observations for data assimilation. As such, this is something we would like to reconsider. Relaxing hydrostatic hypothesis is less of a priority for our applications. However, parameterizations of their effects in an hydrostatic context would be valuable to better represent evolution and mixing associated to resolved internal waves. (Mercator)

Using the Boussinesq approximation as we do now may complicate or degrade the assimilation of altimeter data or the interpretation of sea-level change. We are not sure how important this might be (we're asking for advice on this internally). We do not see non-hydrostatic effects as a priority for our global models. For the NWES, we are not sure at what resolution this could become an issue. We know several NERC academics who use MITgcm rather than NEMO because of its non-hydrostatic capabilities. (Met Office)

Hydrostatic – no. Boussinesq – yes (NOC)

2f. Is the parameterisation of the entrainment into and mixing within the near surface boundary layer particularly important for your applications and sufficiently well represented by NEMO? Is improved representation of mixing deeper in the water column also a priority?

Yes it is important for our applications and for the coupling with biogeochemistry. The representation of mixing deeper in the water column is a priority in particular when tides are explicitly represented. (CMCC)

Inclusion of Langmuir turbulence should be improved. Near surface velocity profiles are greatly impacted by this regime. Non-local effects of Langmuir turbulence are also poorly represented by standard Fickian vertical mixing schemes. (Mercator)

We believe that the parametrisation of the surface and bottom boundary layers is important, particularly in coupled AIWOL models, and are continuing to invest in the OSMOSIS parametrisation which aims to improve it. The representation of mixing deeper in the water column in NEMO has been much improved over the last few years. We are not using these developments in our latest global configurations (GOSI9) but aim to use them in future versions. (Met Office)

Yes, on climate timescales this matters and relates to earlier point about the MOC being too shallow. Realistic diapycnal mixing in the interior ocean is important especially on longer timescales and for mean circulation. (NOC)

2h. Should NEMO's scale-aware parameterisation of the mesoscale and/or submesoscale processes be improved? If yes, what particular aspects should be improved (e.g. impact

on frontal jets or low frequency variability, impact on the shape of the energy spectrum, scale-awareness of the parametrisation)

For our purposes it is important to improve the scale dependent methods (i.e. methods based on machine learning techniques). (CMCC)

In MOI applications large scales are controlled by data assimilation. An improvement of the shape of energy spectrum at high frequency is of interest. We expect that parameterisations in combination with other numerical schemes maximize the effective resolution of the model. (MOI)

We believe this should be a priority (particularly for configurations like ORCA025 which only partly resolve the mesoscale, but also for higher resolution models). We are not in a position to distinguish between the particular aspects cited. The scientific credibility of the schemes is important for us, so all of these aspects could be relevant. But (rightly or wrongly) the overall impact of the scheme is likely to be judged by its impact on the temperature biases and the path and strength of the major current stream (e.g. the Gulf Stream extension or the Azores current). (Met Office)

Yes this is very important as we continue to work at scales (eg ¼) that are (at best) eddy permitting rather than resolving (and analogous issue for submesoscale at higher resoltions). Also important for ocean-shelf and low-high latitude transitions where Rossby radius varies substantially across the model domain. (NOC)

2i. Should NEMO have single or multiple options for parameterisations (recognising the overhead of supporting many options)?

We propose to have multiple choices of parameterizations which should be consolidated and well documented. (CMCC)

The reduction of options should be favoured even if it's complicated for a community code. Another option would be adopting a more generic approaches (vertical physics for example) in order to be able of maintaining a code with a good level of robustness (MOI)

Having multiple (two or three) options where there is real uncertainty (e.g. structural uncertainty) is an important advantage as it allows more robust ensembles of integrations to be constructed. We believe that it should be possible to extend the use of the SETTE system to exercise multiple parametrisation options so that the overhead of supporting carefully modularised alternatives need not be excessive. (Met Office)

Multiple – these are aspects of active scientific research, without yet a consensus on approach. NOC's efforts (in vertical) focus on OSMOSIS and GLS (NOC)

Q3: ICE MODELS

3a. What are your requirements for ice shelves, icebergs and sea-ice?

The coupling between ocean/sea ice with ice shelf and iceberg components is crucial for properly reproducing polar dynamics and the large-scale feedbacks on climate (e.g. Antarctic bottom water formation and Arctic outflows). For global or regional applications in polar regions, a flexible interface with new available codes might be considered. The ISF module in NEMO is a good start but needs a large effort and validation in the near future mainly for a realistic discharge of freshwater in the ocean. The impact of ice sheet/glacier melting in the Northern Hemisphere needs consideration too. (CMCC)

Apart from the effects on the tides, we have not identified any operational applications for ice shelves. We plan to develop iceberg forecasting capacities but we have no experience in the iceberg module yet. The representation of sea ice must meet our commitments in areas such as polar environment monitoring, marine navigation, marine resources and conservation. In other words, the existing ocean indicators for sea ice need to be extended and expanded to include other indicators characterizing sea ice states such as ice volume, snow depths, drift speed, surface temperature, surface albedo and different ice types. Given our goals of increasing resolution, an adequate representation of the MIZ remains crucial for operational systems at such high resolution. The physics of the sea ice has to be compatible with the interactions with marine biogeochemistry. Sea ice must perform well in both Arctic and Antarctic. (MOI)

We require icebergs and ice shelves for climate model simulations but ice shelves are less of a priority for short-range real-time predictions. For short-range real-time sea-ice predictions future requirements are likely to be much more stringent than those for sea-ice climate simulations. For the latter the continuum model formulation is satisfactory. Even though the resolution of the models we run at (i.e., ORCA025) is below the resolution that the sea ice model can resolve properly, its response to ocean/atmosphere forcing at these scales is acceptable. For short-range forecasting, continuum models such as SI3 are considered unsuitable for navigation purposes because they do not directly model the location of leads or floes and are not designed for modelling them in the marginal ice zone (MIZ). To provide more useful products for real-time operations we would likely need to represent floes and leads and may need to consider discrete element modelling - either as part of the continuum model or instead! (Met Office)

3b. Which essential processes are missing and need to be improved for your applications ?

The accuracy of all dynamics processes at high resolution should be revised (as ice strength parameterization). The coupling between sea ice and biogeochemistry is also important. (CMCC)

Given the increasing role played by waves on ice edges, an interface between ice and waves must be clearly established. Although we have so far done very little work on BGC in the polar regions, there is a need to clearly identify which tracers should be represented in the interactions between ice and bgc. (MOI)

To provide more useful products for real-time operations we would likely need to represent individual floes and leads and to better represent marginal ice zone processes. Although icebergs are important for forecasting, the current iceberg scheme in NEMO is not able to meet those demands - being focussed primarily on the climatological distribution of freshwater melting rather than the location of specific bergs. It’s worth noting that in order to do iceberg forecasting properly one would need a good input berg calving/location dataset (which could in theory be used to initialise the model). (Met Office)

(i) Wave mixing in partially/fully sea ice-covered areas. (ii) Ice fragmentation effects might be important in the fully coupled mode with waves and atmosphere, in the forced mode it has moderate local impact. (iii) Maybe internal tides (NOC)

3c. What is the expected performance of the code?

The cost of the advection remains expensive. The entire cost of the sea ice model should not exceed 15-20% of the total cost of the coupled ice-ocean configuration. (MOI)

The sea-ice code needs to perform reasonably well on CPU-based, GPU-based and vector-based HPCs. Whilst its cost is less than 20% of that of the NEMO ocean code its performance is not a major issue. The current iceberg code does not parallelise so does not work effectively on GPU or vector machines. (Met Office)

3d. Should the sea ice model remain closely connected to the ocean component? Is the new SI3 model meeting your institute's needs?

It seems that the use of stand-alone sea ice is not optimal and requires a minimum of coupling with the ocean. The possibility of using a mixed layer coupled with sea ice is very interesting given our high resolution and assimilation objectives. With the new SI3, the ability to activate landfast ice and the activation of aEVP for example are very interesting capabilities for us. The new model already meets a lot of our expectations and we haven't explored everything yet. Given our objectives we expect improvements on: snow representation (assimilation context), surface albedo (to broaden our offer), optimised advection scheme, sea ice rheology (pressure & ridges) and last but not least ice-atm/ice-ocean drags. (MOI)

Yes. The close connection and coupling to NEMO was our number 1 reason for adopting SI3! The current continuum model formulation of SI3 meets our needs for climate scale simulations but is not able to represent the processes required for high-resolution sea ice forecasting and for real-time applications. However this is a general problem for sea ice modelling (see Blockley et al., 2020; Hunke et al., 2020) and not a limitation that is specific to SI3. [https://doi.org/10.1175/BAMS-D-20-0073.1; https://doi.org/10.1007/s40641-020-00162-y] (Met Office)

Yes close connection is important (NOC)

Q4: BIOGEOCHEMISTRY COMPONENT

4a. Is your institution using a biogeochemistry component? If so, for what purposes, aside from strictly biogeochemistry?

At CMCC we develop the Biogeochemical Flux Model (BFM, www.bfm-community.eu) that is coupled with NEMO since version 3.6 and it is implemented in global and regional configurations. The long term strategy is to maintain the coupling interface of NEMO within TOP and sustain the realization of shared interfaces between physics and biogeochemistry. In addition to the purely pelagic biogeochemical components our system links with biogeochemical active fields that are not transported through NEMO, but share an interface with the water column (e.g. a benthic sub-module). (CMCC)

Yes, we are currently using the PISCES model. Aside from strictly biogeochemistry, this model is very useful to highlight some issues with the dynamical component (OCE) including physical data assimilation, and it is used to force higher trophic level models. It is also used to build ocean health indicators to stakeholders, policy makers and environmental agencies. (MOI)

Yes we use ERSEM for shelf-sea predictions and MEDUSA for global climate simulations. We use NEMO-ERSEM to provide information about the lower levels of the food web as well as nutrients, oxygen, pCO_2etc (via CMEMS); in the longer term we are aiming to develop this to provide better representation of other aspects, such as particulate and dissolved organic matter, light attenuation. We would also like to use the models to investigate coupled systems, e.g. the impact of river inputs on eutrophication, atmosphere-ocean transport etc. (Met O)

Yes Earth Systems modelling, coupling to higher trophic level models (NOC)

4b. Do we need a BGC model closely linked to ocean dynamics component?

Actually there are several models coupled to NEMO, so the existing interface with a clearly specified API is the minimal component that enables the coupling of the different biogeochemical systems to the ocean dynamics. (CMCC)

Yes, it is a need from our side. At Mercator, even the people who develop the dynamical component of NEMO regularly plug in the BGC component to test the impact of their developments on the BGC tracers. In current systems, the assimilation of physical data into ecosystem models can cause the deterioration of the biogeochemical simulations due to the breaking of physical balances and of their consistency with the biogeochemical field. A promising approach is the combined assimilation of physical and biogeochemical data to address the above issue and preserve the consistency between the physical and biogeochemical simulations. In particular, using bio-optical modules that provide feedback from biology to ocean physics in "two-way" coupled models are expected to preserve even better such consistency, in both the simulation and assimilation steps of operational systems. The opportunity for the combined assimilation of physical and biogeochemical data is increasing along with the growing number of BGC-Argo floats and gliders mounting multivariate sensors in the ocean. The EU H2020 SEAMLESS project is dedicated to implement PHY-BGC joint assimilation. So, coupled PHY-BGC models are going to be a key point in operational oceanography. (MOI)

We do not see a strong need for this at an application level (we do not use the PISCES model that is within the NEMO system). However there may be good technical drivers for including a BGC model within NEMO (e.g. to ensure that the interface to BGC is working correctly in new model releases or to serve as a concrete example of how to couple a BGC model to NEMO). There are also advantages to including biogeochemistry in at least some parts of NEMO testing: this can flag up issues that may affect biogeochemistry runs later, and can also indicate issue with parameterisations of physical processes, such as vertical transport. (Met O)

Yes especially at high resolution. We use MEDUSA tightly integrated to NEMO, and have found intermediate couplers less efficient or problematic. (NOC)

4c. What are your objectives and needs for grid coarsening?

Grid coarsening will be beneficial for running high resolution configurations with active biogeochemical components. This is so far the main solution to tackle the computational burden due to the physical transport of several oceanic tracers. Alternatively (or complementary) HPC improvements on the physical transport of tracers could speed up computations further reducing the overall cost of having online coupled biogeochemical models. (CMCC)

We currently use the online coarsening capacity that was developed by Clément Bricaud and is on a branch of NEMO3.6. We use it both to output some variables on a coarsened grid and to force biogeochemical model PISCES at a lower resolution. Grid coarsening is a strong need for MOI in the near future. (MOI)
The objective is to use a credible BGC model without increasing the computational cost of the physical model by a large factor (e.g. by more than 50%). UKESM have a strong requirement for grid coarsening to use with MEDUSA. We also want to use grid coarsening of ERSEM in our NWES system. (Met O)

We see this as a 'necessary evil' for running with BGC at even modest resolution (1/4 deg) ESM configurations. The non-linearity in the response of BGC to vertical velocities make this conceptually very problematic. But a robust and sustainable solution is required. (NOC)

Q5: I/O AND DIAGNOSTICS

5a. Does the computational efficiency of the diagnostics code have a significant impact on the model's cost?

The online diagnostics is a very useful tool that reduces the post-processing effort on the model output and improves the accuracy of specific quantities when computed run-time. It has been largely used by CMCC in the CMIP exercise. Anyway, it requires computational time and memory that can be a bottleneck for big configurations and long simulations. The impact on the I/O (via XIOS) is still a limitation for our global high res applications. Possibility to use a different I/O tool instead of XIOS. There are other limitations in the I/O that can be improved for large-domain applications, such as the online interpolation method that might be re-written for big matrices at high frequency (no errors are reported at the moment for these issues). (CMCC)

Future evolution of MOI systems will be depend on the performances of: the "reading" capacity with the increase of resolution of atmospheric forcing (exp: ECMWF/IFS, 1/8° 3-hours to 1/14° 1-hour) the "output" capacity with the increase of resolution and frequency output, and the ensemble approach. Capacity to make diagnostics for ensemble approach. (MOI)

It does in our work-horse configurations partly because a very large number of diagnostics is output. (Met O)

Not sure. I/O itself is definitely an issue. (NOC)

5b. Do you see further application of the obs operator as a priority?

For the moment it is not a priority for CMCC applications. (CMCC)

In the context of complete modularization of the Mercator forecasting and analysis system, it was decided to separate the observation operator from the model and assimilation modules. However, we believe that the IAU (Incremental Analysis Update: a method which smooth the incremental inputs over the analysis window) module should remain in the model. Therefore, there is no priority on the current NEMO observation operator. (MOI)

We use the observation operator in our short-range forecasting and reanalysis suites. It has been used as a preparation step prior to data assimilation and for verification. In order to simplify our internal systems we have stopped using it for verification and may stop using it as a prior step to data assimilation. Other groups within the Met Office, working with simpler sets of observations, have written alternative code to compare model and observations for validation. This may sound inefficient but the overall overheads are probably small. (Met O)

No – we generally prefer off-line tools (python, matlab etc) (NOC)

Q6: AGRIF

6a. What are the target applications for AGRIF in your institution ?

We use AGRIF for regional zooms mostly over the European domain. (CMCC)

Embedded 1/108° zoom in IBI (Iberian Biscay Irish) operational system (1/36°) Multiple zooms in key areas (narrow straits/overflow regions) in our global eddy resolving model. (MOI)

We would like to use it to improve the resolution of ORCA (particularly ORCA025) in key regions such as the Denmark Strait and other overflows, the Mediterranean outflow and the Gulf Stream separation. We might use it more extensively to represent the continental shelf and slope. (Met O)

AGRIF to improve N. Atlantic overflows and in some regional applications. (NOC)

6b. How efficient does AGRIF need to be for the target applications?

Adding an AGRIF zoom without penalizing the cost of the parent model (by adding processors and running both in parallel) would be welcome. This does not seem to fit the existing methodology of mesh refinement but would undoubtedly encourage the implementation of zooms. (MOI)

This depends of course on the benefit from using it. Increasing resolution by a factor of 3 typically increases HPC costs by about a factor of 30. If representing key regions improves the overall representation significantly then it might be acceptable for the overall model to be 3 times as expensive as the mother grid without AGRIF. If AGRIF were deployed in such a manner there would be a focus on making it as efficient as it was feasible to be. There would also be a focus on ensuring that AGRIF could be used “out of the box” in new releases. New releases would need to include SETTE test cases involving AGRIF in ORCA025 using the preferred choices of vertical coordinate systems. (Met O)

Not known yet, but expect load balancing between parent and child grids as a major issue. (NOC)

6c. What interfaces are required for data assimilation with AGRIF?

We are not using AGRIF with data assimilation. (CMCC)

We don’t know the answer to this question. It might be sufficient to perform the data assimilation on the mother grid (particularly if there is only one level of nest used by AGRIF). This would certainly be the first step for implementing data assimilation with AGRIF. If AGRIF was being used to improve resolution in an area important for customers then we might need to implement assimilation at the higher resolution as well. In that case a lot of work would need to be done in the external DA software, and the NEMO OBS and IAU codes would need to work with AGRIF. (Met O)

None (NOC)

6d. Do you see a potential use of AGRIF methodology (e.g. enabling sharing variables on different grids in memory space) beyond grid refinement (ex: coarsening of physics for bgc)?

Our focus application remains the grid refinement (also in vertical). (CMCC)

The AGRIF methodology should be applied to the online, conservative, coarsening of physical variables (for biochemistry modeling in particular). (MOI)

In principle, we believe, either AGRIF or OASIS could be used to perform grid-coarsening. Either option would be acceptable to us. The choice could depend on how to make the best overall use of funding opportunities and staff resources. (Met O)

Not currently (NOC)

Q7. MACHINE LEARNING

7a. What usages do you envisage for machine learning within NEMO (please try to be as precise as possible in terms of timescale and Technology Readiness Level)?

We envisage to enlarge the experience of the atmo community is developing in terms of parameterizations of unresolved processes to the oceanographic community (i.e. mixing, momentum flux). (CMCC)

Refinement of uncertain parameters (ex: BGC modeling); Adding/augmenting/replacing parameterizations (ex: non hydrostatic processes); Downscaling (MOI)

There seem to be several usages. Two obvious ones are: use of high-resolution simulations to train parametrisations in coarser simulations; and use of observations to improve the representation of model bias in short-range predictions and re-analyses. These are new fields that will gradually mature. It seems that there are some relatively easy wins so that initial implementations could be ready for implementation quite quickly and then be gradually replaced by more refined schemes. (Met O)

No active experience in this – but interested conceptually in ML for parameterization. (NOC)

7b. Does NEMO need a specific interface with machine learning and what constraints should there be on an interface?

The development of an interface between NEMO and machine learning approaches largely depend on the applications that NEMO wants to target. The use of ML for pre-processing, coupling with other components, ocean parameterization, forecasting and the analysis of model output might all need different ML methods and different interfaces. (CMCC)

We are not well placed to answer this question. We believe the answer is yes but the interfaces are evolving rapidly and we do not have expertise in them. However we do have strong links with Microsoft, HPE and CRAY so might be well placed to explore their SmartSIM interface functionality in collaboration with others (e.g. Andrew Shao). (Met O)

7c. Are there any specific on-going efforts in your institutions at the interface between scientific computing and machine learning, that you believe could be relevant to NEMO development in this area ?

Several experimentations are in progress at CMCC in using ML for climate and oceanographic studies, as an example:

- Use of ML approach to speedup numerical kernels inside the model. In this regards we are experimenting the implementation of the MUSCL advection process through a LSTM network
- Use of ML approach to enhance SSH prediction near the coast using observations

- Automatic identification of cyclones and prediction of their trajectory by means of CNN networks
- ML approach to detect and forecast marine heat waves and predict short-term Arctic sea ice variability

MOI is building expertise around ML through several collaborations but these sit outside NEMO for the time being. (MOI)

No one in the ocean modelling team in the Met Office has been actively engaged in ML up to this point. There are other groups (e.g. the Infomatics Lab) that might provide advice. (Met O)

Q8: HPC

8a. What is the expected performance of the code that is required for each of your target applications by 2026 (simulated years per day) and approximately how many cores would be used for these simulations?

Considering the Black Sea model developments, we plan to extend the spatial domain to include the Azov Sea online coupled to sea-ice model and the target for the production of reanalysis and near real time (analysis and forecast) datasets is SYPD <= 1 in 2026 considering a maximum number of cores equal to 288. Considering the Med Sea configuration at 1/24 deg resolution and 141 vert levels we expect SYPD < 1 using 252 cores. For the global configuration at 1/16 deg resolution and 98 vert levels we expect SYPD = 1 using 1620 cores. (CMCC)

MOI will use up to 50 000 cores:

- System without DA: Maximum 1 day for 1 year simulated for the global 1/36° configurations or regional 1 km resolution configurations.
- Deterministic system with DA: actually, 3 hours are necessary to make a 7-days cycle with the MOI global 1/12° (forecast run + analyse + hindcast). This performance should be the same with future global 1/36° system.
- Ensemble approach requires running independent members or small set of members. In the second case, we need a smart communication between XIOS and the ensemble members, otherwise the system is very difficult to set up. This is especially true for large configurations such as global 1/12°.

For most applications the number of simulated years per day is quite strongly constrained (e.g. a 5-day forecast has to be delivered by a particular time; a 30-year reanalyses should not take longer than about 6 months to produce). The cores available can be distributed across ensemble members, so low-resolution large-ensemble configurations can be an attractive option. In 2019 we were able to run ORCA0083 reasonably efficiently on about 250 36-core nodes (achieving 2 SYPD) and ORCA025 on 70 nodes (achieving 10 SYPD). We would expect to use at least 6-10 times as many cores (or their GPU equivalent) within the next 6-8 years. (Met O)

ORCA12-N512: At least 2+ years/day, ~20000 cores (NOC)

8b. Do you see flexibility of deployment on different HPC architectures as a high priority requirement?

CMCC is going towards the use of GPU-based architecture. An efficient exploitation of GPUs requires NEMO to be redesigned for a flexible parallelization . (CMCC)

Future HPC architectures will be based on hybrid approach (CPU, GPU, low or high memory node, I/O capacities,...). NEMO should be able to be installed on different HPC architectures. (MOI)

Yes, because we do not know what HPC architectures will be available. We need to be able to run reasonably efficiently on CPU-based machines (similar to current ones), vector machines and GPU-based machines. We may also need to be able to adapt NEMO to other types of machines. We want to be able to achieve this with one unified source code. (Met O)

Yes – we use many configurations on multiple HPC machines. Also flexibility of processor map (non-uniform decomposition) would be helpful for local additional components (– but is complex to implement message passing (POLCOMS has this capability in early 2000's). (NOC)

8c. Do you expect to run a very large model (e.g. global very high resolution) or ensembles of fairly high resolution models, or huge ensembles of lower resolution models or a combination of all three?

CMCC expects to run ocean/ice configurations at (sub)mesoscales and approach a large number of ensemble members for specific applications. In both cases, increasing the HPC performances is a priority.

MOI expects to run all these three scenarios, more precisely we expect to work with:

- Deterministic: global very high resolution (1/12° and 1/36°), regional configuration (1/108°)
- Huge ensemble at low resolution (1/4°) "coupled" with small ensemble at high resolution (1/12°)

We want to be in a position to do all three. Our focus is likely to be on the two ensemble categories (rather than a single very high resolution model). (Met O)

Yes primarily high resolution O-A couple simulations, or high resolution NEMO-BGC. Less interest in huge ensembles of low resolution models. (NOC)

Q9: VERIFICATION AND VALIDATION

Quality control exists for NEMO reference code, for the reliability of developments and releases. Still, improving it appears to NEMO developers as a very high priority, both for the developers and for the users. Quality control covers a number of subjects and methods (documentation, continuous integration, vérification, validation up to unit testing…).

9a. Which of these activities should be given highest priority?

One of the most demanding phases in the development process is the unit test and system testing. An automatic and permanent tool for testing would help. Moreover, monitoring the changes of the computational performance after a code update is relevant for providing the developer with an insight on the impact that its changes have on the code performance. (CMCC)

MOI suggest 2 priorities: a) Validation thanks to tests cases seems the easier and more efficient way. It allows to showcase easily toward users the evolution of the developments. A demonstration based on global configuration including all components seems also essential. ORCA2 is too small/ not enough sensitive ? b) Continuous integration & verification of SETTE tests using gitlab capacities to automatize these tasks which are now handled manually and willingly.

The Met Office's suggested order of priorities for exploration (highest first) is:

- The opportunities offered by gitlab for more continuous integration
- The ideas for making the the SETTE regression testing framework more modular and deploying it so that it covers a wider range of options
- Consideration of the options for a framework for enabling unit testing and easy generation of tabulated diagnostics
- The NEMO documentation might explain better the strategy behind its organisation. This might help developers to get up-to-speed more quickly.

Bug free code – maybe through better approach to unit testing ?? (NOC)

Q10: INTERFACES

10a. What are your requirements for interfaces to other code systems? For example interfaces to data assimilation systems or frameworks (this could include a need for TAM)/ interfaces to BGC models (either for ocean or sea-ice)/ interfaces to atmosphere/other ocean models/waves/interfaces to machine learning

For our applications we would require more modularity of NEMO to improve interfaces with other models especially for climate and ESMs. Our priority is also interfaces with nested models either built with NEMO or other types of models such as unstructured ones. (CMCC)

Maintain all existing interfaces with Oasis and follow Oasis evolutions (if any). Start to test XIOS coupling interface when it will be available (MOI)

We assume this question is intended to ask whether the existing interfaces are satisfactory and whether there are additional interfaces we would like to have. The lack of a grid coarsening interface is certainly an issue (because it's potential is clearly apparent). The "internal" interface between NEMO developers and AGRIF needs to be improved: new developments tend to break AGRIF. A training course and AGRIF guide for NEMO developers might help to resolve this. (Met O)

TAM would be really useful. Interface to wave models (either through coupler (OASIS) or hard-wired) (NOC)

10b. Would you be willing to commit resources to re-establishment of a tangent model for NEMO?

This is not a priority for our institute. (CMCC)

No (MOI)

There is a C3S project proposal in which INRIA propose to update the TAM to a later version of NEMO (we think version 4.0.4) . Longer-term we would like to investigate 4Dvar which requires a TAM but it isn't currently high enough priority to offer resources to do it. The tangent and adjoint models should include model parameters as well as the initial conditions in their control variables. There is a significant group of academics in the UK that use MITgcm because of its TAM capabilities. (Met O)

It would be difficult to priorities this over other activities. Currently it would need independent support from a competitively won science funding. (NOC)

10c. Is there a requirement for grid coarsening in your target applications?

Currently not. (CMCC)

The integration of coarsening in NEMO4 should facilitate the use of a dual resolution data assimilation analysis. Also, in both contexts of very high resolution configuration and of huge ensembles, we expect to output some fields in a coarse resolution grid. (MOI)

Yes, grid coarsening for BGC applications has relatively high priority. (Met O)

Yes (NOC)

Q11: COMMUNITY SUPPORT AND TOOLS

11a. How important is focused support for the academic community?

Enlarging to the academic community may be an added value for NEMO itself and this should be supported through dedicated training activities. (CMCC)

Not sure to understand the question (MOI)

If NEMO is to be a state-of-the-art model its links to the academic community need to be strong and its support for new users/developers (PhD students) needs to be good. The tools for building new configurations are much easier to use now than previously and the information on how to use them has improved. But there may still be a gap here that could be addressed with relatively little effort. (Met O)

Very important for NOC.

11b. Is the scientific documentation of the NEMO code adequate? Should it be given higher priority?

An improved scientific documentation would be an added value for the NEMO community. The documentation (NEMO manual) might be re-structured and homogenized. It should be provided simultaneously with every new release, i.e. all new or modified routines should be described and commented on. To simplify the external pdf document, we might think of adding already a detailed description inside the code in the single routine. The actual form to modify/update/revise the manual documentation is complicated, a quicker procedure/tool may entice developers to proceed on it. Additionally, it can be valuable to have a dedicated documentation platform to collect/track major differences between versions and to describe main innovations introduced in the recent releases. (CMCC)

No. But an online & modern version of the documentation (such as the user guide base on readthedocs) would be a plus. (MOI)

The documentation is very succinct. In places it could perhaps explain the strategy of the code a little more clearly. ECMWF has a small team of people devoted to scientific documentation of their code. It might be worth looking for a member of staff with good writing skills who could work with subject experts to improve the documentation. (Met O)

This should be a high priority, but maybe a more dynamic structure would be appropriate (web site rather than book). (NOC)

11c. Who do you currently turn to for code related problems?

Colleagues in the NEMO System Team. (CMCC)

Internal MOI experts, trac nemo ticket system, new discourse forum (MOI)

Typically other members of the NST. (Met O)

Internal points of expertise and individual personal contacts in the consortium. (NOC)

11d. Would you be willing to share ideas/approaches for training of new members of the NEMO System Team?

We suggest to have a dedicated section on the NEMO website to host presentations and relevant scientific materials for training purposes. (CMCC)

Not sure that Nemo ST team is renewing frequently enough so that it needs a specific training. The simpler solution for new members consists in being trained by the previous ST member. (MOI)

Yes, we think this would be a good idea. (Met O)

Yes (NOC)

11e. Would you be willing to put staff resources into training for NEMO users?

It will be for sure an action to further support and can be eventually considered as part of the actions to propose. (CMCC)

Training Nemo users must be considered as part of nemo ST & devs missions. It also means improving Nemo documentation & user guide, as well as creating new idealized testcases to illustrate model capacities, so it will be valuable for both users and developers. (MOI)

We need to provide training for internal users of NEMO and would be willing to consider doing this in collaboration with other members of the NEMO consortium. (Met O)

Yes, possibly - open to discussing this. (NOC)

11f. Do you think that the current frequency of NEMO releases is about right/too frequent/not frequent enough?

The frequency of NEMO is high based on the effort that we can give to a proper validation of new codes and based on the users' response in updating the NEMO-based systems. More than fixing a 2year time, a strategy to set the release frequency might be based on deliverables in the strategic plan. From an operational point of view, a frequent (less than 2 years) update of the code version is not applicable considering the time needed to update the configuration, test and validate it in a long term period. (CMCC)

One major release over a few years (2 years between 4.0 and 4.2) + multiple minor bugfixes releases per year seems ok (MOI)

The frequency of merges (as opposed to releases) could be more frequent now that we have more experience with 6-monthly merges and remote merges. The frequency of releases should be determined by progress on new functionality rather than a pre-set timetable. New releases should have had some scientific validation (which is resource intensive), in addition to SETTE testing, and be accompanied by releases of updated documentation. A release every second year would be about right. (Met O)

Q12: CARBON FOOTPRINT

12a. Did your institution compute its annual carbon footprint for the past years? If yes, for which year(s)?

Yes MOi computed its annual carbon footprint for year 2019, and also for years 2018 and 2020 as far as HPC is concerned. (MOI)

Yes in 2019/2020 (and subsequent years) (Met O)

Yes, we have done so for a number of years. (NOC)

12b. What is the percentage of computing (order of magnitude) in each of these annual evaluations?

In 2019, HPC represented 35% of the footprint, knowing that only 3 other pillars were taken into account (professional travels; daily home-office commuting; consumptions linked to our building like electricity, air-conditioning or heating). It is worthy to note that between 2018 and 2020, the carbon footprint of the single HPC pillar **grew by 40% each year**. (MOI)

The percentage of computing that year was estimated to be 35% (46 million kWhours for both operation and cooling which translated to 12 000 tCO2e). (Met O)

Not known. (NOC)

12c. Is your institution engaged in reducing its carbon footprint?

Yes the commitments has been taken, but detailed plans are not defined yet (in discussions). (MOI)

Yes, we have corporate level targets and a serious commitment to reducing our footprint. We have targets for reducing travel (e.g. by 8% this FY). It is stated that our HPCs will use renewable sources of electricity (which have a slightly reduced CO2e tariff: 1kWh =0.18 kgCO2e for renewable electricity compared with 0.23 kgCO2e for standard electricity). (Met O)

Yes, we lead a netzero oceanography exercise (NOC)

12d. Is the carbon footprint of your applications using NEMO going to be a driver to design the future? If yes, with which metrics?

We are working on this and once metrics are completed we will share with the Consortium. (CMCC)

It may be. We have not considered this properly yet. (Met O)

Yes, it will influence our model design and practices. (NOC)

2.2 Reducing NEMO's carbon footprint

2.2.1 Context and motivations

Successive IPCC reports have clarified the role of human activities on the Earth's climate and their consequences. Following the Paris Agreement, our governments are now committed to reduce global emissions by 55% by 2030 in order to keep global warming below 2°C.

In our working communities, the +1.5 IPCC Special report has crystallised the perceptions of a number of us. Since this report, a number of evaluations of Carbon Footprint in our work have started, and been annually updated. Some decisions have been made or are underway at each level (from governments to institutions, research labs, professional communities) in order to set our working pratices in line with this energy transition required by the announced trajectory (-55% in 2030).

2.2.2 Objectives

Some people believe that research and development activities can/should stay out of this reduction/transition processes, be an exception. We are convinced of the opposite: as experts contributing to the IPCC reports and/or the understanding and forecasting of Earth's oceans and climate, we are convinced we must give example, and demonstrate the coherency between the knowledge we produce, the conclusions of IPCC reports, and our working practices. This appears to us as a need for our intellectual coherency, our mental health, and our scientific legitimacy. Moreover, if there is going to be decisions made on all working activities to reduce carbon Footprint, we believe that we, as scientific experts of the domain, are in a good position to elaborate propositions allowing both the energy transition and the preservation of our ability to produce and disseminate knowledge. Our approach here aims to be scientific, as in our work: at first evaluate the Carbon footprint of NEMO (its development and its use) and identify its contribution to the Carbon Footprint of our working activities. From there, in the perspective of a transition towards reduction of Carbon Footprint, we intend to elaborate some possible ways for the future.This section aims at bringing together some relevant ideas and possible drivers for the future of NEMO: its development so as its applications.

2.2.3 Initial Evaluation

A large number of organisation have started to evaluate their yearly Carbon Footprint. It is becoming a duty in many countries now. Concerning our work, there is no formal sharing of this important information yet. Our first hypothesis here is to believe that we (NEMO developers and users) are mostly functionning on the same basis in terms of energy and resources consumption. As a "first guess", we propose to examine the Carbon Footprint of the LOCEAN research lab in Paris in order to identify the order of magnitude of the different sources of carbon emission.

- 2018 Carbon Footprint of LOCEAN :https://climactions.ipsl.fr/wp-content/uploads/2020/07/empreinte_co2_labo_update_2020-2.pdf
- 2019 Carbon Footprint of LOCEAN https://climactions.ipsl.fr/wp-content/uploads/2021/06/bilan_2019_LOCEAN.pdf
- A synthesis of the different contributions to Carbon Footprint at LOCEAN, based on 2018 evaluation: https://climactions.ipsl.fr/wp-content/uploads/2020/07/infographie-climactions-v8-scaled.jpg

A few noticeable elements from these first evaluations include:

- The total carbon footprint of LOCEAN in 2018 is 1750 teCO2 in 2018, so that the yearly Carbon Footprint at work per person in the lab is 9.5 teCO2. Knowing that the transition to reach in 2030 should bring each citizen to limit its Carbon Footprint (work and personal) to 2 teCO2, our carbon Footprint at work clearly needs to be reduced
- Travels are the main contribution in 2018 : not far from 50%. Within this contribution, 97% concerns travels by plane and in those, 80% concerns long distance flights. This analysis demonstrates that this part is a very good candidate for reduction, and as a consequence LOCEAN has decided to set individual yearly quotas for travels: starting at 12 TeCO2 per person in 2020 (a lot!), and progressively reducing each year.
- More global studies on this sort of reduction now happening in many places show that setting travel limitations does allow about an overall 25% reduction of Carbon Footprint in our working activities.
- Once this reduction is underway, the other contributions increase in percentage of the total, and as so, deserve attention. On this aspect, numerical modeling is then a relevant part to examine. Some numbers: if we consider a round trip in plane Paris-New-York as a unit (= 2teCO2), then CMIP6 at LOCEAN counts for 41, a 10 years simulation of NEMO global configuration at 1° resolution counts for 1/100 and at 0.25° resolution for 1/4. Choosing what should be CMIP7, or a spatial resolution for NEMO simulations are indeed significant and important choices...

2.2.4 Available options as drivers for NEMO development

- Optimize NEMO (HPC WG) in order to do the same things with less Carbon Footprint, or to do more with same Carbon Footprint (rebound effect)
- Machine learning as an option to explore and choose at reduced energy cost the best parametrizations and their configuration
- More developments on AGRIF (coarsening, adaptative AGRIF zooms...)
- Innovate on the methodology to develop NEMO in a collaborative fashion (also requested by time zones span by future consortium, if it includes non-european institutions)

2.2.5 Available options as drivers for the applications using NEMO

- Use AGRIF to avoid setting high resolution everywhere
- Define and use new metrics combining the gain in terms of science and the energy cost increase (e.g. for example what is actually improved when switching to higher resolutions? Is the cost bearable?). The metrics should evaluate costs versus benefits regarding the science produced by NEMO so as the way the results are used (using or moving large amounts of data being also a problem). As a start, this publication could be of interest : "CPMIP: measurements of real computational performance of Earth system models in CMIP6" https://gmd.copernicus.org/articles/10/19/2017/

- Better elaborate the extreme runs and share efficently (including evaluation of storage and data moving costs in terms of energy) the products of the NEMO simulations in the community, in order to avoid duplications
- Develop online courses and tutorials so as to accompany new or existing users in their applications of NEMO, optimizing their learning hence minimizing the production of un-necessary (aka wrong) simulations

2.2.6 What's next?

Create a NEMO Working Group on these questions related to many different aspects of NEMO development and use, in order to elaborate on mid term possible solutions?

3 Ocean model Kernel

WGLs: Mike Bell, Florian Lemarié and Gurvan Madec

3.1 Introduction

3.1.1 Assessment of the 2018-2022 Development strategy

The main issues discussed in the 2018-2022 strategy were

1. the vertical grid
2. the horizontal grid
3. the time-stepping algorithm

The focus in that period has been on the introduction of a Runge-Kutta (RK) time-stepping algorithm (through the EC funded IMMERSE project). A significant change to the time-indexing of the model fields was made to enable more flexibility in the time-step scheme and analyses made of the stability of options for efficient time-stepping of the external mode (Ducousso et al 2021). Good progress is being made implementing a 3rd-order RK scheme and it is expected to become available in vn 4.2.1. Further work to refine the methods used, in particular to explore compensated space-time schemes, will continue as business as usual.

Relatively little progress has been made on the vertical co-ordinate. However assessments of the dependence of diapycnal mixing on various schemes (including z-tilde coordinates) and parameter settings in realistic global configurations have been made (Megann et al. 2020) and the scoping study envisaged in the strategy has made useful progress over the last 12 months. The Brinkmann penalisation method (Kevlahan et al. 2015, Debreu et al., 2020) has also started to emerge as an elegant and powerful approach for representing small-scale variations in bathymetry (and potentially embedded sea-ice and ice shelves). Such approach is relevant for a z-coordinate model as it eliminates some artefacts due to the step-like geometry.

A "lesson learnt" here is that it is probably unrealistic to expect to work on more than one major aspect of the code formulation within a 5-year period.

The previous strategy noted what were then relatively new formulations for hexagonal and triangular horizontal grids using either finite element or finite volume methods. The MPAS and FESOM teams are exploring these approaches. As a group we don't have expertise in these issues and the impacts of making such changes on other aspects of the code would be very wide ranging. Our view is that code using such grids would constitute another model. A smoother representation of the "side" boundaries could be achieved instead by (nearly) terrain-following coordinates. There may be merit in using the alternative meshes for estuarine models, but that is not the main focus of the NEMO consortium members. So we will not discuss alternative horizontal grids in more detail.

3.1.2 Priorities for the 2023-2027 Development strategy

The outstanding issues on which we would like to make progress in the next 5 years are

1. Generalised vertical coordinates with vertical ALE (V-ALE) algorithm
2. Better representation of bathymetry-flow interaction processes
3. Green computing: improving the energy efficiency of NEMO

The expected benefits from a physical viewpoint are the reduction of spurious diapycnal mixing in the ocean interior (particularly in climate simulations), the improvement of the flow over sills as well as of the steering of the flow by the bathymetry. For example, there are some suggestions that the rapid degradation of Gulf Stream separation in the first phases of spin-up depends on representation of the bathymetry (Ezer 2016; Schoonover et al. 2017). Another illustration of the detrimental effect of the step-like representation of the bathymetry is that the discretisation of the Coriolis term gives rise to a false representation of the forces on gyre circulations (Styles et al. 2021).

3.2 Vertical grids and representation of bathymetry

3.2.1 Generalised vertical coordinates (VLR vs V-ALE vs Quasi-Eulerian)

A very educational description of vertical Lagrangian remapping (VLR), arbitrary Lagrangian Eulerian (V-ALE) and quasi-Eulerian schemes is provided in Griffies et al. (2020).

The VLR method uses a Lagrangian approach to advection in the vertical combined with an Eulerian approach in the horizontal. This requires a directional splitting. In standard implementations of directional splitting the order of integration is permuted at each time-step to reduce splitting errors (e.g. Strang splitting). Since there is no such permutation in VLR implementations it can be at most first-order accurate and cross-derivatives terms can lead to stability issues depending on the time-stepping (Lemarié et al. 2020). Within the ALE framework these problems can be avoided because standard 3D advection can be used and stability issues associated with vertical advection could be handled via the Shchepetkin 2015 approach. More general V-ALE formulations in which the movement of the target grid is not purely Lagrangian appear to be attractive.

The specification of the target grid is a major challenge: one can specify isopycnals as the target grid or penalise departures from isopycnal slopes and grid smoothness as in Hofmeister et al (2010) or Gibson (2019). Alistair Adcroft has noted that it is very hard to find a globally satisfactory set of isopycnal target surfaces. More generally, the difficulty is that the choice of a satisfactory target grid corresponds to the resolution of an optimization problem jointly under 1D (e.g. sufficient resolution in boundary layers, avoid vanishing layers, etc) and 3D (e.g. regularity of vertical levels) constraints.

Some of the results obtained by Alex Megann (in Megann et al (2020) and subsequently) with z-tilde coordinates are somewhat puzzling: increasing the viscosity, using z-tilde and 4th order rather than 2nd order fct horizontal advection each reduce diapycnal mixing but only by about 10-15%; 4th order vertical advection has relatively little impact. Some caution is needed interpreting these results as they were obtained with the leapfrog scheme and a very specific choice of numerical options (e.g. very low viscosity values see Holmes et al 2021). Also there is not a clear consensus on how to quantitatively diagnose diapycnal mixing. These results should not stand in the way of developing more generic vertical coordinates but suggest that the effectiveness of schemes in reducing diapycnal mixing will need thorough evaluation.

Along the way, schemes for the horizontal pressure gradient (hpg) force specifically designed for the presence of sloping layer geometries, nonlinear equation-of-state and non-uniform vertical stratification profiles would also be required (Shchepetkin & McWilliams, 2003; Adcroft et al., 2008; Engwirda et al., 2017). It should also be decided whether the hpg force should assume that tracer values are cell-mean values (which would make the pressure forces less smooth) and how to reduce hpg errors due to the dependence of density on depth (Shchepetkin & McWilliams 2003).

3.2.2 Brinkman volume penalization for representing complex geometry

Brinkman penalisation is a method to implicitly enforce boundary conditions for complicated or moving geometries through the addition of specific source terms to the continuous dynamical equations. With this method the solid boundaries are treated as a porous medium whose representation depends on permeability and porosity parameters. In Debreu et al, 2020 it is shown that the total energy of the penalized primitive equations can not increase (stability) and that constants are preserved (consistency). Moreover, at a discrete level, the method does not introduce any new stability constraints. There are several possibilities to choose the Brinkman penalization parameters (permeability and porosity). A possibility is to consider a smooth (envelope) terrain following (generalised) coordinates with more rapidly varying bathymetry (lost during the smoothing procedure) represented using porosity and permeability settings. The approach also allows to eliminate the step-like detrimental effects associated with z-coordinates. It should however be noted that a lot of effort is required to specify the penalization parameters in a systematic way for a high resolution, large area model.

The methodology has been implemented in the Croco ocean model in both idealized and realistic settings. In particular, unpublished results by Laurent Debreu show improved Gulf Stream separation at 0.25° resolution. There is also potential to represent ice-shelves with penalisation and embedding sea-ice in the ocean by using a time-varying penalisation.

3.3 Energy efficiency

Nowadays, given the increase of energy costs and the need to adopt environmentally friendly practices, model developers must deal with a new technological paradigm to keep under control the carbon footprint of numerical simulations. The (time/energy/cost)-to-solution for a given effective resolution is an increasingly important metric to evaluate a given numerical code (e.g. Kalinnik et al, 2021). Besides the software environment, important drivers affecting the energy-to-solution are directly related to the dynamical kernel and include the time-integration strategy as well as the dissipative/dispersive properties of numerical schemes. The environmental constraint on oceanic dynamical kernels thus necessitates to re-assess existing algorithmic strategies (Mengaldo et al., 2019) and to keep a technological watch on hardware evolution.

From this perspective the evolution from leapfrog to RK time-stepping goes in the right direction: the effective resolution is improved, the code runs ~50% faster and there are no tuning parameters like the one associated to the Robert-Asselin filter. Several initiatives around the NEMO kernel could be envisioned to help for a responsible use of the code:

→ More systematic evaluation and documentation of the cost vs benefits of the particular options available in the code (in particular for vertical physics and advection schemes). The more expensive schemes can serve as a reference.

→ Closer collaboration with the HPC WG to determine which algorithmic choices fit the best on given architectures.

→ Thinking in terms of effective resolution vs computational cost, following Sanderson (1998) it is beneficial (and even optimal) to use third or fourth order schemes (however such study would deserve to be updated).

3.4 Additional issues

The following points have been raised during the preliminary discussions on the development strategy. The first two points (relaxing the Boussinesq and/or the hydrostatic assumptions) are mentioned because there are frequent questions about their feasibility and the extent of the associated developments.

3.4.1 Hydrostatic Boussinesq/Non-Boussinesq options

It is often considered that non-Boussinesq (hydrostatic) equations could be easily used by virtue of the isomorphism between the z-coordinate Boussinesq and pressure-coordinate non-Boussinesq systems (DeSzoeke & Samelson, 2002). However such isomorphism exists only under the rigid-lid assumption and does not directly apply to modern oceanic models based on a mode-splitting algorithm with a prognostic free-surface. Another possibility, following Greatbatch et al., 2001 is to replace the discretized vertical volume factor $\rho_0 \Delta z$ by $\rho \Delta z$. Relaxing the Boussinesq assumption also requires the use of full dynamic pressure in a fully compressible, realistic EOS (acoustic waves being still excluded via the hydrostatic assumption). Generally speaking, the Boussinesq assumption removes several interdependencies within model components (e.g. it filters out conversion between internal and kinetic/potential energy) and it is not as straightforward as it seems to relax it (Shchepetkin & McWilliams, 2011). As a first step, a thorough understanding of Shchepetkin & McWilliams 2011 and of the non-Boussinesq formulation in MOM6 seem necessary.

3.4.2 Non-hydrostatic option

The implementation of a non-hydrostatic option within an existing hydrostatic ocean model has profound implications for the code: either the use of an external library to solve efficiently the corresponding 3D elliptic boundary value problem in the Boussinesq (incompressible) case or the integration of a (very) fast acoustic mode in the non-Boussinesq ("pseudo" compressible) case. The "pseudo'' compressible approach is implemented in the CROCO model (Auclair et al., 2018) which uses an additional super-fast level of time-step splitting for the 3D acoustic mode and is very efficient on massively parallel architectures. Such a fast 3D mode allows to integrate other terms raising stability/accuracy issues, e.g. bottom friction, vertical advection, non-traditional Coriolis terms. Overall this is a major undertaking in terms of development and the cost vs benefits ratio given the typical NEMO user requirements is unclear.

The possibility of moving to an AGRIF mother-child interface with the CROCO code could be considered as a potentially viable alternative to developing an internal NEMO NH capability. Another possibility instead of resolving explicitly NH effects would be to parameterise them. There are ongoing initiatives to use machine learning techniques to do so.

3.4.3 Physics/dynamics coupling

The consistency between the kernel & parametrisations particularly for the transfer of energy between resolved and sub-grid scale forms should be borne in mind (e.g. Burchard 2002; Marsaleix et al. 2008, Eden et al 2014). TKE and GLS do this whilst OSMOSIS does not. A broader reflection on physics/dynamics coupling is provided in Gross et al. (2018).

3.4.4 Unintrusive developments

An improved scheme for momentum advection TVD, monotonicity-preserving or WENO (as well as for tracers) is desirable to regularize the velocity field with an expected reduction of numerical diapycnal mixing.

The Shao et al (2020) isopycnal diffusion scheme can simply slot in as an alternative option.

A form of biharmonic GM based on the Greatbatch & Lamb (1990) vertical mixing of momentum formulation is being developed. Again this should be relatively unintrusive.

Only the vector invariant form for surface wave - mean flow interactions has been coded up (Couvelard et al., 2020). Implementing the flux form given by Couvelard et al (2020) is relatively straightforward (unintrusive). The Bennis et al 2011 test case should be implemented.

3.5 References

Adcroft, A., R. Hallberg and M. Harrison (2008). A finite volume discretization of the pressure gradient force using analytic integration. *Ocean Modelling* 22, 106-113.

Auclair F., L. Bordois, Y. Dossmann, T. Duhaut, A. Paci, C. Ulses and C. Nguyen (2018): A non-hydrostatic non-Boussinesq algorithm for free-surface ocean modelling, *Ocean Modelling*, Volume 132

Bennis A. C., F. Ardhuin and F Dumas (2011): On the coupling of wave and three-dimensional circulation models: Choice of theoretical framework, practical implementation and adiabatic tests. Ocean Modelling Volume 40, Issues 3–4, Pages 260–272 http://dx.doi.org/10.1016/j.ocemod.2011.09.003

Burchard, H.(2002): Energy-conserving discretisation of turbulent shear and buoyancy production. *Ocean Modelling* - 4. 347-361.

Couvelard, X., F. Lemarié, G. Samson, J.-L. Redelsperger, F. Ardhuin, R. Benshila and G. Madec: Development of a two-way-coupled ocean–wave model: assessment on a global NEMO(v3.6)–WW3(v6.02) coupled configuration, Geosci. Model Dev., 13, 3067–3090, (2020)

Debreu, L., N. Kevlahan and P. Marchesiello: Brinkman volume penalization for bathymetry in three-dimensional ocean models. *Ocean Modelling*, 145, (2020)

de Szoeke, R. A. and R.M. Samelson: The duality between the Boussinesq and non-Boussinesq hydrostatic equations of motion. J. Phys. Oceanogr. 32, 2194–2203 (2002).

Ducousso N., F. lemarié, L. Debreu and G. Madec (2021): Stability and accuracy of Runge--Kutta-based split-explicit time-stepping algorithms for free-surface ocean models. *Journal of Advances in Modeling Earth Systems* (in review)

Eden, C., Czeschel, L., and Olbers, D. (2014). Toward energetically consistent ocean models. *J. Phys. Oceanogr.* 44, 3160–3184. doi: 10.1175/JPO-D-13-0260.1

Engwirda D., M. Kelley, and J. Marshall (2017): High-order accurate finite-volume formulations for the pressure gradient force in layered ocean models, *Ocean Modelling*, 116.

Ezer, T. (2016): Revisiting the problem of the Gulf Stream separation: On the representation of topography in ocean models with different types of vertical grids. *Ocean Modell.*,104,15–27.

Gibson A.: An adaptive vertical coordinate for idealised and global ocean modelling*, PhD thesis, Australian National University,* (2019)

Greatbatch, R. J. and K.G. Lamb (1990): On Parameterizing Vertical Mixing of Momentum in Non-eddy Resolving Ocean Models, *Journal of Physical Oceanography*, *20*(10), 1634-1637

Greatbatch, R. J., Y. Lu and Y. Cai (2001) : Relaxing the Boussinesq Approximation in Ocean Circulation Models, *Journal of Atmospheric and Oceanic Technology*, *18*(11), 1911-1923

Griffies, S., A. Adcroft and R. Hallberg (2020): A Primer on the Vertical Lagrangian-Remap Method in Ocean Models Based on Finite Volume Generalized Vertical Coordinates. *Journal of Advances in Modeling Earth Systems*. 12.

Gross, et al. (2018): Physics–Dynamics Coupling in Weather, Climate, and Earth System Models: Challenges and Recent Progress, *Monthly Weather Review*, *146*(11), 3505-3544

Hofmeister, R., H. Burchard and J.-M. Beckers: Non-uniform adaptive vertical grids for 3D numerical ocean models. *Ocean Modelling*, 33. 70-86. (2010)

Holmes, R. M., J. D. Zika, S. M. Griffies, A. McC. Hogg, A. E. Kiss and M. H England (2021): The Geography of Numerical Mixing in a Suite of Global Ocean Models. *Journal of Advances in Modeling Earth Systems*, 13, e2020MS002333. https://doi.org/10.1029/2020MS002333

Kalinnik, N., R. Kiesel, T. Rauber, M. Richter and G. Rünger (2021): A performance- and energy-oriented extended tuning process for time-step-based scientific applications. *The Journal of Supercomputing*.

Kevlahan, N. K. -R. and Dubos, T. and Aechtner, M. (2015): *Adaptive wavelet simulation of global ocean dynamics using a new Brinkman volume penalization. Geosci. Model Dev., 8, 12, 3891--3909.*

Lemarié et al. (2020): *D3.1 - Algorithm specification and code design for 2LTS scheme,* IMMERSE Deliverable

Megann, A. and D. Storkey (2021): Exploring viscosity space in an eddy-permitting global ocean model: Is viscosity a useful control for numerical mixing? *Journal of Advances in Modeling Earth Systems*, 13

Marsaleix, P., F. Auclair, J.-W. Floor, M. Herrmann, C. Estournel, et al. (2008): Energy conservation issues in sigma-coordinate free-surface ocean models. *Ocean Modelling*, 20 (1), pp.61-89

Mengaldo, G., A. Wyszogrodzki, M. Diamantakis, S.J. Lock, F. Giraldo and N. Wedi (2019): Current and emerging time-integration strategies in global numerical weather and climate prediction.*Arch. Comput. Method E.* 26, 663-684

Sanderson, B. G. (1998). Order and Resolution for Computational Ocean Dynamics, *Journal of Physical Oceanography*, *28*(6), 1271-1286

Schoonover, J., Dewar, W. K., Wienders, N., & Deremble, B. (2017). Local Sensitivities of the Gulf Stream Separation, *Journal of Physical Oceanography*, *47*(2), 353-373

Shao, A., A. Adcroft, R. Hallberg and S. Griffies (2020): A General-Coordinate, Nonlocal Neutral Diffusion Operator. *Journal of Advances in Modeling Earth Systems*. 12.

Shchepetkin, A.F. and J.C. McWilliams (2003): A method for computing horizontal pressure-gradient force in an oceanic model with a nonaligned vertical coordinate. *J. Geophys. Res.* 108, C3, 30390.

Shchepetkin A.F. and J. C. McWilliams (2011): Accurate Boussinesq oceanic modeling with a practical, "Stiffened" Equation of State, *Ocean Modelling*, Volume 38, Issues 1-2

Shchepetkin A.F. (2015): An adaptive, Courant-number-dependent implicit scheme for vertical advection in oceanic modeling, *Ocean Modelling*, Volume 91, 2015, Pages 38-69.

Styles, A., M. Bell,l D. Marshall, D. Storkey (2021): Spurious forces can dominate the vorticity budget of ocean gyres on the C-grid. Submitted to JAMES.

4 Parametrisation of eddy closures

WGLs: Andrew Shao and Chris Wilson

4.1 Introduction

4.1.1 Assessment of the 2018-2022 Development Strategy

The previous strategy identified as a key oceanic parameterised physical process, "the representation of the impact of balanced turbulence (mesoscale and submesoscale eddies) on larger scale/lower frequency flows […] this field of research is very active […] with several new approaches […] (scale aware closures, stochastic closures, energy backscatter, approaches from LES)[...]". It also proposed the striking of a Eddy Closure Working Group (ECWG), which first met in September 2021.

4.1.2 Goals and objectives of the working group

A primary goal of the working group is to determine what eddy closures would situate NEMO as an appropriate oceanic model for the types of applications that the community anticipates to be using. While of some of these applications have sufficient resolution to resolve the mesoscale, it is unlikely that global simulations especially those used for climate will be feasible due to their computational expense- for example resolving the mesoscale on the coastal shelves and/or the Arctic would require O(1km) resolution. Thus, parameterizations of meso- and submeso-scale turbulence are crucial to the continued use of NEMO for these types of simulations.

This working group has tacitly agreed that the current suite of parameterizations in NEMO is in line with other GCMs, but has identified a need to add additional schemes for applications whose resolution is in the so-called eddy-permitting regime. The existing suite is likely to be overly diffusive/dissipative in these cases and/or exclude some eddy processes all together.

Lastly, it has been communicated that sharing and testing parameterizations across the community is somewhat ad-hoc. Part of this arises from the high barrier to entry to include new code in the main NEMO trunk. This working group will make a recommendation for a more community-oriented framework that is complementary to the existing core NEMO development workflow.

4.1.3 Synergistic activities within the broader oceanographic community

(DRAFT NOTE: This has been preliminarily been discussed by the chairs and partly within the working group, but has not yet been tabled for full discussion and debate)

Significant coordinated efforts are underway both within Europe and the United States (via the Eddy Energy Climate Process Team) to both suggest new eddy parameterizations and also develop idealized test cases to evaluate. The WG will evaluate the current state of these efforts and determine what can be adapted for use in NEMO.

4.2 Metrics and indicators for prioritization

4.2.1 Scientific Objectives

The working group has identified a number of processes and biases that are common to most non-eddy resolving global simulations. The list provided below is by no means novel nor unique to NEMO specifically, but serves as a motivation to judge whether new parameterizations are likely to improve these high priority items.

- Better representation of jets (e.g. Gulf Stream extension and Azores Current)

- General need to increase kinetic energy in eddy-permitting models
- Biases in AMOC variability
- Weak climate variability and ensemble spread
- Southern Ocean eddy saturation and eddy compensation (the latter may be the more important for heat and carbon transport and budgets) in non-eddying models.
- Isopycnal structure near surface and bottom boundaries (sensitive to GM tapering)
- Biases in ocean heat uptake particularly for projecting changes under climate change
- Choice of degree to which eddies mix along neutral surfaces, i.e. tapering at the surface and bottom boundaries

4.2.2 Prioritization indicators

At this stage, the working group is primarily meant to be advisory as opposed to directing work and research. The following considerations were taken into account when recommending which existing parameterizations and promising research directions should be prioritized for uptake into NEMO

- What are the fundamental 'needs' vs. 'wants' for the immediate applications being pursued within the Consortium?
- Is the barrier to implementation sufficiently low to allow for implementation within the timeframe of the strategic plan?
- Can the skill of the parameterization be tested against the scientific objectives listed in Section 2a?

4.3 Recommendations of parameterizations for inclusion

(DRAFT NOTE: These parameterizations have not been prioritized, but comprise closures under consideration by the WG)

4.3.1 Under development within the NEMO community

The following parameterizations have been implemented in the community, but have yet to be upstreamed into the main NEMO trunk

- Biharmonic operator for Gent-McWilliams
- Prognostic eddy energy-based scheme following the GEOMETRIC framework[1-3]

4.3.2 Implemented in other models

The following have been implemented and demonstrated in other models (listed in parentheses)

- Energization of the mean flow by the eddies, i.e. backscatter[4-7] (FESOM, MOM6)
- Leith-based viscosity[8,9] (MITgcm, MOM6)

4.3.3 Known eddy effects with no existing parameterization

4.4 Implementation strategy

(DRAFT NOTE: To be discussed)

4.5 References

1. Marshall, D. P., Maddison, J. R. & Berloff, P. S. A Framework for Parameterizing Eddy Potential Vorticity Fluxes. *J Phys Ocean.* 42, 539–557 (2012).

2. Mak, J., Marshall, D. P., Maddison, J. R. & Bachman, S. D. Emergent eddy saturation from an energy constrained eddy parameterisation. *Ocean Model* 112, 125–138 (2017).

3. Mak, J., Maddison, J. R., Marshall, D. P. & Munday, D. R. Implementation of a Geometrically Informed and Energetically Constrained Mesoscale Eddy Parameterization in an Ocean Circulation Model. *J. Phys. Oceanogr.* 48, 2363–2382 (2018).

4. Juricke, S. *et al.* A Kinematic Kinetic Energy Backscatter Parametrization: From Implementation to Global Ocean Simulations. *J. Adv. Model. Earth Syst.* 12, e2020MS002175 (2020).

5. Jansen, M. F., Held, I. M., Adcroft, A. & Hallberg, R. Energy budget-based backscatter in an eddy permitting primitive equation model. *Ocean Model.* 94, 15–26 (2015).

6. Jansen, M. F., Adcroft, A. J., Hallberg, R. & Held, I. M. Parameterization of eddy fluxes based on a mesoscale energy budget. *Ocean Model.* 92, 28–41 (2015).

7. Klöwer, M., Jansen, M. F., Claus, M., Greatbatch, R. J. & Thomsen, S. Energy budget-based backscatter in a shallow water model of a double gyre basin. *Ocean Model.* 132, 1–11 (2018).

8. Leith, C. E., Stochastic models of chaotic systems, *Physica D.*, *98*, 481-491, 1996.

9. Bachman, S. D., Fox-Kemper, B., and Pearson, B. (2017), A scale-aware subgrid model for quasi-geostrophic turbulence, *J. Geophys. Res. Oceans*, 122, 1529– 1554.

5 Surface fluxes and vertical mixing

WGL: Guillaume Samson

5.1 Introduction

In order to improve air-sea interactions in Nemo, 4 priorities have been identified during the last NDS plan:

- representing feedbacks between the OSBL and the ABL
- improving turbulence closures in the OSBL
- more sophisticated bulk schemes
- representing wave-current interaction processes

We propose to keep those same priorities for the next NDS to structure and prioritize new developments.

5.2 Representing feedbacks between the OSBL and the ABL

To address the first point, 2 solutions have been implemented in Nemo:

- a parameterization of the surface current effect on the wind stress following Renault et al. 2020 has been implemented in the bulk formulae. This scheme uses a linear relationship between the wind forcing and the surface stress from an observation-based statistical regression to compute a correction coefficient that mimics the dynamical coupling. This scheme uses standard 10m-wind forcing to be activated.

- an atmospheric boundary layer model (ABL1d) following Lemarié et al. 2020 has also been implemented. ABL1d is a single-column model with a vertical discretization of the lower atmosphere. It allows an explicit representation of both dynamical and thermodynamical coupling between OSBL and ABL by solving the air temperature, humidity and wind evolutions through vertical mixing and sea-surface boundary conditions. Contrary to the Renault et al. parameterization, ABL1d needs additional external fields (3D atmospheric forcings) in order to relax the model toward the atmospheric forcing.

Concerning future evolutions related to OSBL-ABL coupling, the following developments have been identified:

- concerning the ABL1d model, only vertical mixing process is represented for now. The so-called pressure adjustment process will be added in order to represent all processes involved in OSBL-ABL coupling.

- an alternate “3D” version of the ABL model including horizontal advection will be developed. It will allow to decrease the relaxation applied to the model and to obtain a model solution in better agreement with oceanic surface conditions. Dealing with coastal lateral boundary conditions will require special care.

- the last proposed development is related to the ABL model, but also more generally to the way atmospheric forcings are read by Nemo and to the HPC WG:

- new atmospheric forcing datasets such as ERA5 and JRA55-DO have strongly increased their spatial and temporal resolutions, as well as the data volume to be read. This is even more the case with the ABL model which needs 3D atmospheric forcings. For now, these data are read sequentially by

Nemo, which can slowdown the code up to 50%. We propose here to use XIOS to read these atmospheric forcings in an asynchronous way, and hence to speed up substantially Nemo.

5.3 Improving turbulence closures in the OSB

To address the second point, 3 solutions have been implemented in Nemo:

- a new vertical mixing parameterization OSMOSIS (ref to add)

- a new implementation of the wave-related mixing effect on the TKE scheme (Couvelard et al. 2019)

- a new EDMF scheme has implemented to parametrize specifically the oceanic convection (Giordani et al. 2021)

Concerning future evolutions related to turbulence closures in the OSBL, the following developments have been identified:

- OSMOSIS scheme development will continue (mainly optimizations and code cleaning)

- Developments started during last NDS and related to Langmuir-circulation induced mixing, its representation in TKE scheme and its potential coupling with wave models will be continued.

- EDMF scheme only support QCO for now (but not yet VVL option). The scheme will also be adapted to work with BGC model and to transport vertically momentum.

Comparison with LES simulations will also be carried to improve the scheme calibration. This LES-comparison methodology could be applied to other vertical mixing schemes in order to verify their performances and compatibility.

- a parametrization to represent mixing induced by near-inertial waves will be developed.

- following previous NDS plan, an attempt to reduce the number of vertical mixing schemes in order to facilitate code maintenance and testing will be made. In particular, it should be possible to mimic the TKE scheme using an appropriate GLS scheme configuration.

However, some simple mixing schemes such as the Richardson one are still used by some institutions and can be useful for debugging purposes or idealized testcase validation. They should consequently be conversed in the code.

5.4 More sophisticated bulk schemes

To address the third point, several developments have been made:

- bulk algorithms implementation have been completely refactored to be in phase with the Aerobulk external package (Brodeau et al. 20XX)

- new bulk schemes have been introduced in addition to the historical one (CORE):

COARE 3.0, COARE 3.6, ECMWF and ANDREAS

- a cool-skin & warm-layers scheme (ref) has been added to COARE and ECMWF bulks

- 3 new bulks schemes over sea-ice have been implemented (only constant coefficients were available before): Andreas 2005; Lupkes 2012 and Lupkes & Gryanik 2015

One additional bulk scheme is proposed for the next period:

- reintroduce the MFS bulk scheme (Castellari et al. 1998) using the new bulk framework

A new parameterization of the wave-age dependency of the Charnock parameter has been proposed and tested in Sauvage et al. 2020. It could be easily included in the actual bulk framework.

In order to simplify bulk related code structure and to limit its size, an interesting approach proposed by Gryanik et al. 2021 (which can be seen as an equivalent of GLS framework for bulk schemes) will be explored.

In link with the SI WG, a bulk mixed layer scheme equivalent to the one included in CICE will be developed in order to represent sea-ice – ocean interactions without using the full ocean model.

5.5 Representing wave-current interaction processes

To address the point 4, multiple novelties have been implemented in Nemo:

- new generic coupling interface between Nemo and wave models (WW3, WAM)

- new wave-induced terms (Stokes-Coriolis, vortex & wave-induced pressure forces) in Nemo equations (only “vector invariant” form for momentum equations) & boundary conditions

- new Stokes drift vertical profile

- wave-effect on TKE vertical mixing scheme (shear production term, wave-breaking surface energy injection, length scales dependency to way surface roughness, new Langmuir turbulence parameterization)

Concerning future evolutions related to wave-current interaction processes, the following developments have been identified (wave-ice related developments are addressed in the sea-ice section):

- new wave developments related to shallow water / coastal will be done, including wave-induced bottom pressure and Stokes drift profiles adaptation to shallow-water environments. But a “limit” must be fixed to these developments depending on the target applications (coastal, littoral, surf zone, …) that Nemo development want to address.

- actual wave developments only available in vector form will be adapted to flux form formalism in order to be usable with more dynamical options.

- the coupling interface (including the Stand-Alone-Surface mode) has become increasingly big and complex due to the multiple components that Nemo has to deal with. A cleaning/splitting of this part of the code will be undertaken to facilitate Nemo coupling with new external components.

- wave induced mixing in GLS vertical mixing scheme following Kantha & Clayson 2004 or Harcourt 2014 (with separated eddy-viscosities for Stokes shear and current shear in the TKE equation).

6 Sea-ice

WGLs: Martin Vancoppenolle and Ed Blockley

6.1 Introduction

The representation of sea ice is important for various purposes (geophysics of sea ice, ocean and climate simulation, operational applications). NEMO now has a single sea ice model named SI_3 (Sea Ice modelling Integrated Initiative), which will be based on the best of its predecessors (LIM3, CICE and GELATO).

The SI^3 model uses a fairly standard continuum model formulation, components and physics, following principles introduced by the AIDJEX consortium in the 1970’s (Coon et al., 1974). It is based on the assumption that sea ice can be represented as a 2+1D continuum drifting under the influence of friction to air, sea and seafloor, Earth rotation, and internal forces. Internal forces assume that sea ice exhibits plastic behaviour (i.e., permanent deformation after a sufficient stress is applied) (Hibler, 1979), using the aEVP method (Kimmritz et al., 2017). The subgrid-scale ice thickness distribution is resolved using ice categories, each of which has specific state variables (for snow and sea ice). 2D horizontal transport equations are used to move state variables around and redistribute them in thickness space; with a specific source/sink term designed to represent physical processes, which can be mostly considered as vertical. Vertical physics include sea ice growth and melt, cooling and warming, brine inclusion dynamics, radiative transfer, and many other parameterisations. Surface albedo is a function of surface state, in particular of melt-pond area and thickness, tracked following the approach of Flocci and Feltham (2007). For the most part, SI_3 is a sea ice model compliant with the state-of-the-art, and with representation processes identified as important by the sea ice community.

The strengths and limitations of continuum sea ice models such as SI_3, along with prospects for their evolution, are detailed in Blockley et al. (2020) and their suitability for operational forecasting applications is discussed in Hunke et al. (2020). These two publications summarise outcomes of a community workshop organised by the NEMO Sea Ice Working Group (SIWG) in Laugarvatn, Iceland, in 2019. In these papers, it is argued that:

1) The continuum model formulation is still very good for describing the large-scale/average behaviour of sea ice and will likely remain relevant for lower resolution and climate studies for many years to come. Continuum sea ice models agree well with current observations and will remain useful for the coming years to decades.
2) Continuum models are not fully appropriate for high-resolution and operational applications, which mean that alternative model formulations may be beneficial for operational forecasting needs in the near future:
    i. Continuum models do not seek to represent features at the grid-scale, such as individual leads, floes or ridges, only the statistical average behaviour
    ii. At high resolution the continuum assumptions can be invalidated because grid-cells do not necessarily contain a representative sample of sea ice floes.
3) Discrete-element models, whose formulation principles are potentially well suited for operational forecasting needs, offer an exciting alternative to the continuum approach, but are not yet mature enough for implementation in large-scale ocean modelling systems such as NEMO.

In this context, we propose here a strategy for the evolution of SI^3, mostly based on the maintenance and development of the current continuum approach, but allowing research on possible alternatives such as DEM. We split our strategy along three main axes: documentation; modularity and interface to Earth System Model components; representation of sea ice processes.

The difficulties that are faced share similarities with the ocean but are also somehow specific to the sea ice. In common with the ocean, SI^3 developers face specific demands from different sub-communities of users, in terms of target resolution, processes, and output diagnostics. One specific aspect of sea ice is that its physical understanding is far less advanced than that of the ocean. Governing equations are under debate (we have only a few "rules") and increasing sea ice model resolution does not necessarily lead to a better representation of the sea ice medium. In particular, it should be stated that sea ice continuum models are mathematically similar to the standard continuum formulation used to derive the Navier-Stokes equations for Newtonian fluid flow. However, the continuum assumption is much more easily invalidated for sea ice because the sea ice floe, the analogue of a molecule in the ocean continuum, is of comparable size to the grid cell used for numerical simulation.

6.2 Main known issues

a. **Documentation.** There is a strong need for documentation to facilitate the uptake of SI3 users. The current documentation is only an advanced draft and so this will need to be progressed as a top priority.
b. **Modularity and interfaces.** Primary users' needs do not directly relate to model physics, but rather relate to interfacing the sea ice code with other codes/systems. A modular code structure is the best approach to allow users the capability to run SI3 with their specific applications.
c. **Representation of sea ice physical processes.** Model physics/numerics in several areas of the code could be improved. On-shelf operational solutions are rarely readily available. Physical understanding is more often the key limitation to progress, just ahead of low staff resources.

6.3 Plan for issue development

a. **Write and review documentation** (IS-ENES, SIWG, Dec 2021). Activities required: (i) Report on model physics, code organisation, structure, etc. in a documentation document; (ii) Evaluate the code and document model performance in a paper; (iii) Improve inline comments within the SI3 code.

b. **Improve modularity and interfaces**
Code modularity and interfaces are important to allow users to easily use SI3, which will increase uptake of the model. Some specific issues include:

   i. **Reduced ocean physics**
   Issue: Many sea ice users need a reduced-complexity ocean (mixed layer).
   Plan: Implement bulk mixed layer from CICE (U. Reading, 2021), which paves way to more advanced schemes, likely out of the SIWG activities.

   ii. **Splitting thermodynamics and dynamics**
   Issue: Some applications would benefit from a full split of ice dynamics and thermodynamics, in order to run sea ice on a separate grid, and benefit from finite-element/volume high-order methods (e.g. DG).

Plan: Allow full separation of thermodynamics and dynamics, and adjust the surface module accordingly (CNRS, 2021).

iii. **Wave-ice interactions**

Issue: There is no clearly identified interface between sea ice and waves within NEMO, although ad-hoc pieces of work have been performed in the past without much coordination. In Brest the wave-divergence term of the momentum equation (and possibly other things) have been done. NOC has implemented collisional rheology (Aksenov). Full floe size distribution (FSD) is possible but implies large extra complexity in the code and is expensive. There are basically 2 groups of stakeholders, with different foci and interests. The WAVE research community members are interested in the effect of sea ice on waves (attenuation, reflection, …). The SEA ICE research community is interested in the effects of waves on sea ice (floe breaking, wave divergence, …).

Resolution: Launch a specific discussion with stakeholders (Reading, NOC, Waves-WG, SIWG, SASIP). 2 objectives: Identify current status of the wave-ice interface and define a strategy for wave-ice interactions that are agreeable to both waves and sea ice stakeholders. This task may benefit from a targeted workshop.

iv. BGC-ice interactions

Issue: The interface with tracers, in particular those used for ocean biogeochemistry (BGC), is rudimentary in the SI3 code. There has been some work done outside of the NEMO workplan to provide specific functionality, however. For instance, Hayashida and Steiner (CCCMa, Victoria) have implemented an ice algae model in NEMO 3.6. Iron in sea ice, treated as a volume tracer in ice categories, has been implemented by CNRS (Person et al., GBC 2020).

Resolution: Launch a specific discussion group with stakeholders (TOP-WG, SIWG, Victoria, CNRS). 2 problems. Define a generic strategy for tracers. Identify whether specific tracers should be incorporated and/or are needed (iron, isotopes, …)

v. **Snow on sea ice as a separate medium**

Issue: There are various advanced continental snow models (CROCUS, SnowTherm, ...). Model infrastructure is not ready to receive them, as snow is intrinsically into the sea ice model. If we want to benefit from such models, there could be a need to introduce a specific interface between sea ice and snow.

Resolution: Revise the snow-sea ice interface to better separate the two media. Interested stakeholders could be identified, in order to introduce more advanced snow models (CNRM?).

vi. **Ice-atmosphere interface**

Issue: Some ice-atmosphere interfaces (e.g. CNRM, CMCC) are not yet fully supported in the SI3 code.

Resolution: Interface suggestions should be sourced from the relevant groups (CMCC, CNRM). Those groups might be helped by using existing NEMO functionality to run SI3 as a separate executable coupled through OASIS. We have to see how deep an involvement of sea ice developers this requires.

c. **Representation of sea ice**

i. **Overarching model assumptions**

Issue**:** Current 1+2D continuum approach is designed for large-scale sea ice modelling at scales of approx. 100 km over days to months. Although it is therefore still ok for climate modelling purposes, it is not fully applicable to the 1km scales relevant for operational forecasting. Although there is no readily available alternative, discrete element (or hybrid discrete-continuum) model approaches do offer promising avenues for future research.
Resolution: Explore **discrete element** approaches (UKMO/NERC). Follow and get in contact with the many groups planning developments in that direction (UWa, Poland, SASIP).

ii. Ice dynamics

- **Sea ice rheology**
  Issue: Which sea ice rheology(ies) is (are) the most appropriate for climate or operational forecasting applications is an open question. SI3 currently contains the EAP and EVP rheologies.
  Resolution: Implement VP rheology and inter-compare plastic rheologies, with a particular focus on operational application (IMMERSE). Provide input regarding a brittle rheology with damage mechanism (SASIP).

- **Sea ice strength**
  Issue: Sea ice strength is highly influential and subject to large uncertainty but only the most basic strength formulation from Hibler (1979) is available in SI3.
  Resolution: Implement the "ridging" formulation of sea ice strength proposed by Rothrock (1975), which is available in CICE (UKMO, work plan 2021).

- **Horizontal transport**
  Issue: Advection remains expensive. Only the Prather '86 scheme is fully satisfactory. FCT4 is not performing as well numerically speaking. The incremental remapping from CICE has to be adapted to the NEMO grid to work. For these reasons, adding more tracers is not easy, which will mean cost implications for BGC, FSD and snow model developments.
  Resolution: Identify interested developers and researchers to progress.

- **Drags**
  Issue: Ice-atm/ice-ocean drag coefficients, do not yet conform to state-of-the art (Tsamados).
  Resolution: UCL has routines in NEMO3.6, which need to be ported into the code at v4.2.

- **Iceberg-sea ice interactions and Antarctic land-fast sea ice**
  Issue: Antarctic land-fast ice does not currently emerge from model physics and may be important for modelling coastal polynyas and dense water formation. An ad-hoc solution has been proposed by van Achter et al. (submitted to Ocean Modelling), combining tensile strength and large icebergs as part of the sea ice mask. However, as this approach requires observations of large icebergs to be available, it is not yet easy to implement globally.

Resolution: Implement grounded iceberg mask for sea ice model. Explore more generic parameterization of iceberg-sea ice interactions for large-scale implementation (UCL/CNRS).

iii. Ice physics

- **Optics**
  Issues: (i) There are questions on the current surface albedo scheme (thickness dependence of albedo). (ii) The Lebrun et la. (2019) transmittance-scheme leads to spurious surface melt reduction. (iii) Assumptions on under-ice spectral distribution of light are wrong. (iv) There exist more sophisticated optics schemes available in other sea ice models (e.g., CICE).
  Resolution: (i) Resolve disagreement on albedo scheme and amend current scheme (CNRS/Reading). (ii) Updating Lebrun et al. (2019) scheme for light attenuation with latest developments. Test multi-layer snow scheme as a solution for excess surface melt (iii) Revise infrared absorption and light fractionation under sea ice (ocean). (iv) Start discussions regarding further developments. Current broadband scheme could be revised. Two-band and delta-Eddington schemes have been introduced in CICE, but what the advantages are of these approaches is not fully clear. Therefore, we need a preliminary evaluation before we move on.

- **Melt ponds**
  Issue: Some melt pond processes are missing (under-ice ponds, refreezing)
  Resolution: Developments are ongoing in Reading (under-ice melt ponds, melt pond refreezing) and should get back reasonably soon into NEMO.

- **Salt dynamics**
  Issues: Schemes from Rees-Jones and Worster (2014) and Griewank and Notz (2013) were identified as best options by Thomas et al. (2020). However, for implementation, one would need to provide an implicit scheme, otherwise we will need to keep sub-time stepping.

- **Thermodynamic core**
  Issues: Thermodynamic phase composition formulas are inconsistent throughout the code (permeability, brine salinity, …). The linear liquidus assumption has implications everywhere. Non-linear liquidus and more general enthalpy approach would be more precise and allow for easier implementation of minerals, frazil ice, platelet ice (as per Wongpan et al., 2021). Three steps would be required: (i) fully expand the code to an enthalpy-based formulation; (ii) Rewrite heat equation with enthalpy basis; (iii) Implement various liquidus formulations. Possible compatibility with TEOS-10 (as per Vancoppenolle et al., 2019).

- **Snow on sea ice**
  Issue: Snow formulation in SI3 is very simple and a constant snow density is used.
  Resolution: Easy progress is to implement the vertical density distribution by Lecomte et al. (UCL, work plan 2021).

6.4 Other issues

i. There are not many test cases for sea ice.
ii. Data assimilation has been used with NEMO sea ice for several decades but is now becoming more popular with non-operational users. SI3 currently has access to the standard assimilation tools in NEMO, maintained by the DAWG, including the observation operator in ‘OBS’ and incremental analysis update (IAU) code in ‘ASM’. The core data assimilation codes however (such as NEMOVAR) are developed and maintained separately outside of NEMO. We need to liaise with the DAWG to ensure there are appropriate links between the ICE and OBS/ASM codes.
iii. We also have a few external tools (evaluation, etc…). How should they be shared and maintained?

6.5 Summary

Progress in the documentation, modularity, and interfacing of SI3 is in the interest of most. Current SIWG members can do part of the job, with the help of the NEMO system team. In some cases, there is a need to link with other WG’s or contact external people.

Physical progresses in the representation of sea ice will occur in the next five years. Our progress will largely be conditioned by our capacity to enrol experienced developers. An optimal organisation of the work among the different developers should be sought for.

7 Land ice / Ocean interactions

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Priority categories definition:

Category 1: this category includes the thematics/topics we think are critical with some resources already planned or proposal planned or submitted.

Category 2: Will be very welcome within 5 years.

Category 3: Relevant but for later.

Category 0: Discussed but ruled out.

7.1 Scope

The different ice forms of the land ice have an important and diverse influence on the ocean (Schloesser et al. 2019; Bronselaer et al. 2018). Most NEMO applications including polar regions must consider the fresh water inputs from land ice melting carefully. Therefore, the development of NEMO involves significant work on the representation of the interaction between land ice and ocean.

The land ice includes ice sheets, icebergs, and ice-shelves. Land ice / ocean interactions includes **ice-shelves**, **glacier termini** and **icebergs** melting, as well as **surface** and **sub-glacial runoff** from the ice sheet.

Land ice builds up through the accumulation of snowfall over Greenland and Antarctica. Seen from the ocean, land ice takes the form of melting **ice-shelves** or **glacier termini** at the edge of the continents, calving **icebergs** that slowly drift at the ocean surface or again seasonal **surface** or **subglacial runoff** induced by ice sheet surface melting **(Fig. 1)**.

Icebergs in NEMO are handled through the ICB module. Surface runoff is handled through the runoff module. Both are included within the Surface Boundary Condition (SBC) code. Basal ice-shelf melt is handled through the ISF module. Both of these are relatively new developments within NEMO.

Although land ice and sea ice bear some physical similarities, the modelling components to handle them are usually drastically different, because the scales of the problem and processes at plays are fundamentally different.

We need a summary schematic of all the processes at play in the strategy. Katherine can help for the schematic. Below example from Nowicki et al. (2016), Jenkins et al. (2016) and Joughin et al., (2012) for inspiration. See end of the document.

This chapter is designed for application going from Earth System Model (ie at least Ocean / Atmosphere / Ice sheet coupled together) to ocean global and regional configurations (with static ice or with a coupled ice sheet model) forced by atmospheric forcing. The horizontal resolution considered in this document spans from 50 km to 1 km.

7.2 Ice shelves

Ice sheet mass loss accounts for around a third of the present rate of global mean sea level rise, and this contribution is expected to increase and eventually dominate global mean sea level change in the coming decades and centuries (Oppenheimer, M. 2019). Importantly, ice sheet mass change is also persistently the most uncertain term in the future global mean sea level budgets (Oppenheimer, M. 2019). It is thus important to understand the physical detail of how ocean and ice sheet interact together. Accurate representation of these interactions is therefore necessary to either adequately capture the physics of the sub-ice boundary layer, water circulation and transport within the ice shelf cavity if permitted by the model resolution or adequately parametrized these interactions if the whole (or part of) the ice shelf cavities are missing.

Ice shelf cavity parametrizations: Category 1

Most global climate models, such as the ones used in CMIP6 do not resolve ice-shelf cavities at all. Therefore, the entirety of ocean / ice shelves interactions needs to be parametrized. Several parameterisations of varying complexity have been developed in the last 20 years to derive melt rates from far-field ocean properties. However, assumptions in the various formulations differ, giving rise to a large variety of melt (Favier et al. 2019). In the latest version of NEMO, only (Beckmann and Goosse 2003) is available and its performance is known to be poor (Favier et al. 2019 and Burgard et al., in prep.). The evaluation of the various ice shelf parametrization in a realistic test bed made by Burgard et al., (in prep) will help to define the few promising parametrizations to be adapted, implemented and tested within NEMO. Such parametrization could also benefit 'cavity resolving' configurations to include the contribution of part of the cavities poorly represented such as area close to the grounding line for example.

Key paper: Burgard, C.; N. Jourdain; R. Reese; A. Jenkins; P. Mathiot: An assessment of basal melt parameterisations for antarctic ice shelves, 2021, in preparation.

Sub-ice boundary layer parametrizations:

As detailed in Asay-Davis et al. (2017), the current ice shelf melt formulation suffers from many deficiencies and lack of knowledge. Preliminary results from ISOMIP+ (Asay-Davis et al. 2016) raised the issue that current treatments of sub-ice-shelf thermodynamics do not converge with vertical resolution, either within a given model or between models. Different choices about how T, S, heat, and freshwater fluxes are treated in the sub-ice-shelf boundary layer led to disagreements between models and a lack of convergence within a given model with increasing vertical resolution. Recommendation on how to achieve such convergence with increasing resolution, changing vertical coordinates will be welcome to achieve more robust science. In the latest flux formulation, ice shelf melt is proportional to the top friction velocity so melt rate is very sensitive to the drag, surface roughness and tides (Gwyther et al. 2015; Hausmann et al. 2020; Jourdain et al. 2017). Knowledge on these key parameters needs to be improved. About the core of the current melt formulations, latest idealized studies shows that the top boundary layer consist of an inner, friction-dominated boundary layer and an outer geostrophic flow, with buoyancy playing a dominant role in both (Jenkins 2016). This double-layer structure is not accounted for in the current sub-ice-shelf / ocean parametrization. A turbulent closure scheme would however be needed before such scheme could be applied to realistic problems. These questions are open research questions and some work is underway with MITgcm. **Category 1**

Key paper: Asay-Davis, X.S., Jourdain, N.C. & Nakayama, Y. Developments in Simulating and Parameterizing Interactions Between the Southern Ocean and the Antarctic Ice Sheet.*Curr Clim Change Rep* **3,** 316–329 (2017). https://doi.org/10.1007/s40641-017-0071-0

Similar approach to the one used to represent ice shelf / ocean interaction cannot be used for vertical ice face. The typical horizontal length scale of the buoyant plumes along a vertical ice face (~10 m) is far smaller than the model horizontal resolution considered in this chapter (~ 1km to ~50 km). Thus, present day regional and global configuration do not have sufficient resolution to capture the ice sheet / ocean interactions at play on glacier termini (ice shelf front or marine glacier). These interactions and the ocean circulation they trigger need to be parametrized. (Cowton et al. 2015; Jenkins 2011; Slater et al. 2016; Rignot et al. 2016). However, it is not clear yet what is the most adequate choice of parametrization for NEMO. So before to implement any of these solutions, we recommend a detailed analysis of performance of what is available, what is needed and at what NEMO resolution these parametrizations are relevant. Having such parametrization for Greenlandic glacier termini will also benefit the ice shelf / ocean interaction communities by its potential application to the vertical ice shelf front. **Category 2**

Coupling with an ice sheet model: Category 1

Despite the limitations mentioned above, models with ice shelf/ocean interaction have advanced to the point where they are being used not only in hindcasts or sensitivity studies with static ice shelf, but also in Earth System Model with evolving geometry based on the response of an ice sheet model to ice shelf melt and surface mass balance (Smith et al. 2021). These tools will be of great helps to estimates future contribution of Antarctica to sea level rise. In NEMO, an asynchronous ice sheet / ocean coupling method is implemented and has been successfully used in various configuration (Favier et al. 2019; Smith et al. 2021; Pelletier et al. 2021).

Two points need a careful evaluation. First, migration of the calving front is allowed by this method but need to be tested in realistic configuration to test its stability and the coherency with the iceberg module. Then, by construction, the procedure used to move the ice shelf draft and grounding line is significantly non-conservative. This issue could be critical for climate application. An option is available to correct the model state in order to remove any trend created by the coupling method. However, this scheme has only been tested in idealized test cases. So, it needs to be tested and evaluated in realistic applications.

To mitigate the conservation limitation and to allow a high frequency coupling, synchronous ice sheet / ocean coupling method are available in the literature (Jordan et al. 2018; Goldberg et al. 2012). However, we (chapter's authors) suggest to not engage any work on the synchronous coupling method as long as a detailed evaluation of the available method is made and ongoing work on this at BAS show encouraging results.

Key paper: Smith R.S., Mathiot P., Siahaan A., Lee V., Cornford S.L., Gregory J.M., Payne A.J., Jenkins A., Holland P.R., Ridley J.K., Jones C.G., Coupling the U.K. Earth System Model to dynamic models of the Greenland and Antarctic ice sheets, J. Adv. Modeling Earth Systems, accepted, (2021) https://doi.org/10.1029/2021MS002520

Possible overlaps/dependencies: wave working group, sea ice working group, vertical mixing, tides, vertical coordinates, machine learning

7.3 Icebergs

Ice sheet acceleration has increased the flux of icebergs over the last 30 years, which will accelerate further in future. Icebergs have been included as Lagrangian particles in several ocean models (review in Asay-Davis et al. 2017) and have been shown to significantly impact the intrusions of CDW towards ice shelves (Bett et al. 2020) and the Southern Ocean in general (Schloesser et al. 2019). However, the influence of these changes cannot be assessed because current iceberg models are based on overly simple physics, with little consideration of links between icebergs and ice-shelf thickness, bathymetry or sea-ice stress.

Calving and distribution: Category 2

In NEMO, the distribution and rate of calving is prescribed as a forcing. The physics of the calving itself is poorly understood and improving it outside the scope of this document. This being said, the fresh water distribution from iceberg melting is very dependent of their size distribution (Stern, Adcroft, and Sergienko 2016). Furthermore, most of the volume is included into the largest icebergs (Tournadre et al. 2016). So, it is critical to be able to represent large icebergs. Calving of such large icebergs is rare and quasi-random. It is not adapted to the current iceberg generation scheme. Once such icebergs generated, a fragmentation scheme (England, Wagner, and Eisenman 2020; Bouhier et al. 2018) is needed to avoid an excessive life time and unrealistic melt pattern (Bouhier et al. 2018).

Dynamics: Category 1

The dynamic interactions between icebergs and surrounding sea ice is essential to reproduced observed trajectory pattern. Lichey and Hellmer (2001) suggest a formulation of the sea-ice force that include free drift of iceberg in low concentrated area and locking of icebergs in the sea ice pack. This formulation was more recently included in the FESOM ice-ocean model (Rackow et al. 2017) and already tested in NEMO (Marson et al. 2018).

On shallow bank, field of isolated grounded icebergs are critical to represent landfast ice (supported by Olason (2016) with isolated islands) and polynyas in their lee side (Massom et al. 1998; 2001; Nihashi and Ohshima 2015). Experiments with crude representation of grounded icebergs show large improvement in the representation of landfast ice, pack ice and polynya representation (Huot et al. 2021; Bett et al. 2020). A landfast ice scheme is already available within NEMO (Lemieux et al. 2016) with sea-ice keels as anchor points. Modification of this scheme will be needed to add iceberg keels as extra source of anchor points. Thus, the realism of iceberg triggered landfast ice is highly dependent of the realism of the grounded icebergs fields. Therefore, work is needed to improve the realism of the iceberg generation (size distribution, thickness, calving sites …) and the grounding scheme (see Vaňková and Holland 2017).

Thermodynamics: Category 1

Recent works show that the plume generated along the sidewall of an icebergs has different regime depending on the background velocity relative to the plume velocity: attached (meltwater is channeled directly to the surface and 'shield' the icebergs) or detached (meltwater is mixed over a broader layer). Each regime drives different melt and leads to different impact on ocean stratification and upwelling of nutrient (FitzMaurice, Cenedese, and Straneo 2017). The meltwater being injected only in surface, the distinction between the two regime is not available in NEMO. Futhermore, we estimates the canonical various iceberg melt formulation (wave erosion, lateral and basal melt) from (Gladstone, Bigg, and Nicholls 2001) need a thoroughly analysis.

Performance: Category 1

During the development of the latest version of NEMO (4.2) it has been stressed a potential issue of performance of the iceberg modules. The total cost of the lagrangian icebergs model depends only of the total number of icebergs (controlled by the calving rate and melting rate), so the coarser the model resolution is, the larger the relative cost of the icebergs model compare to the total cost of a simulation is. First analysis of the iceberg performance carry out by MetOffice shows that the icebergs code is entirely serial and not performant on CPU as well as on GPU. It probably requires a re-write of the linked-list logic. Furthermore, by nature, there is a large load balance issues between the 'iceberg domains' and the others. Finally, the icebergs modules have not been tested within AGRIF and icebergs cannot cross AGRIF and BDY boundaries.

Key paper: Asay-Davis, X.S., Jourdain, N.C. & Nakayama, Y. Developments in Simulating and Parameterizing Interactions Between the Southern Ocean and the Antarctic Ice Sheet.*Curr Clim Change Rep* **3,** 316–329 (2017). https://doi.org/10.1007/s40641-017-0071-0

Possible overlaps/dependencies: Wave working group, Sea Ice working group, vertical mixing.

7.4 Runoff

It is known that the emergence of fresh subglacial runoff at glacier or ice sheet grounding lines generates buoyant turbulent plumes that enhance heat transfer across the ice–ocean boundary and the submarine melt rate for the portion of the glacier face (Jenkins 2011) or ice shelf (Wei et al. 2020) in direct contact with the plume. It is also a key process in the fjord ocean dynamics (Gladish et al. 2015) and in the transport of nutrient to the surface (Hopwood et al. 2018). Furthermore, estimates of the subglacial runoff for the Greenland (still very uncertain for Antarctica) are now available using regional atmospheric model (IMOTHEP project). However, most of global models (NEMO included) neglect the input of subglacial runoff because of the lack of data or because model capability to inject fresh water in depth are missing. **Category 1**

It is worth noting that, mostly for Greenland, because of the resolution of the targeted configurations, most of the Fjords where the Greenlandic Marine Glacier sit cannot be explicitly represented. So, the modeled circulation, fresh water inputs (glacier melt, icebergs melts, ice mélange) within a 2D (x-z) fjords needs to be evaluates. If it appears such simple representation is not fit for purpose, such fjords will need to be parametrized. **(Category 3)**

Key paper: Gladish, C. V., Holland, D. M., Rosing-Asvid, A., Behrens, J. W., & Boje, J. (2015). Oceanic Boundary Conditions for Jakobshavn Glacier. Part I: Variability and Renewal of Ilulissat Icefjord Waters, 2001–14, Journal of Physical Oceanography, 45(1), 3-32. Retrieved Sep 19, 2021, from https://journals.ametsoc.org/view/journals/phoc/45/1/jpo-d-14-0044.1.xml

Possible overlaps/dependencies: Ice Shelf section of Land Ice strategy, vertical mixing.

7.5 Wider model developments:

Since a couple of years, NEMO has included more and more test cases for evaluation, development and debugging purposes. The land ice / ocean interaction is not well represented in theses test cases (only few capabilities are tested). To assist the development of the land ice /ocean interaction in the future we strongly encourage developers to develop and implement a test case with any development made on this topic (icebergs, ice-shelf, coupling, tide water glacier …). **Category 1**

In the future, NEMO will include new representation of the interaction between bathymetry and ocean using a penalization method. As mentioned in the conclusion of Debreu et al. (2020), this method could lead to some improvement in the representation of ice shelves cavities. However, this is a long-term feature. It is still at the test case stage and will probably not be mature enough within the next 5 years (ie not beyond the period cover by the strategy). Our position is to wait it is mature enough and that any benefits from penalization method will be welcome in the representation of subgrid scale bathymetry feature, ice shelves and ice sheet coupling. **Category 3**

Furthermore, based on the first preliminary results, the proposal submitted we are aware of, Deep Learning based parametrization of ocean / land ice interactions will likely be developed and evaluated against more conventional parametrization. Therefore, potentially (depending on the comparison outcome) there will be a need of an interface to send data in/out between NEMO and a Deep Learning environment such as SmartSim (Partee et al., n.d.) to use such parametrization within the NEMO framework. If relevant, development of such an interface is out of the scope of the Land Ice / Ocean interaction chapter and should be address to the HPC working group or Machine learning working group. **Category 3**

Possible overlaps/dependencies: Kernel/HPC strategy

7.6 Bibliography

Asay-Davis, Xylar S., Stephen L. Cornford, Gaël Durand, Benjamin K. Galton-Fenzi, Rupert M. Gladstone, G. Hilmar Gudmundsson, Tore Hattermann, et al. 2016. "Experimental Design for Three Interrelated Marine Ice Sheet and Ocean Model Intercomparison Projects: MISMIP v. 3 (MISMIP +), ISOMIP v. 2 (ISOMIP +) and MISOMIP v. 1 (MISOMIP1)." *Geoscientific Model Development* 9 (7): 2471–97. https://doi.org/10.5194/gmd-9-2471-2016.

Asay-Davis, Xylar S., Nicolas C. Jourdain, and Yoshihiro Nakayama. 2017. "Developments in Simulating and Parameterizing Interactions Between the Southern Ocean and the Antarctic Ice Sheet." *Current Climate Change Reports* 3 (4): 316–29. https://doi.org/10.1007/s40641-017-0071-0.

Beckmann, A, and H Goosse. 2003. "A Parameterization of Ice Shelf–Ocean Interaction for Climate Models." *Ocean Modelling* 5 (2): 157–70. https://doi.org/10.1016/S1463-5003(02)00019-7.

Bett, David T., Paul R. Holland, Alberto C. Naveira Garabato, Adrian Jenkins, Pierre Dutrieux, Satoshi Kimura, and Andrew Fleming. 2020. "The Impact of the Amundsen Sea Freshwater Balance on Ocean Melting of the West Antarctic Ice Sheet." *Journal of Geophysical Research: Oceans* 125 (9): 1–18. https://doi.org/10.1029/2020JC016305.

Bouhier, Nicolas, Jean Tournadre, Frédérique Rémy, and Rozenn Gourves-Cousin. 2018. "Melting and Fragmentation Laws from the Evolution of Two Large Southern Ocean Icebergs Estimated from Satellite Data." *The Cryosphere* 12 (7): 2267–85. https://doi.org/10.5194/tc-12-2267-2018.

Bronselaer, Ben, Michael Winton, Stephen M. Griffies, William J. Hurlin, Keith B. Rodgers, Olga V. Sergienko, Ronald J. Stouffer, and Joellen L. Russell. 2018. "Change in Future Climate Due to Antarctic Meltwater." *Nature* 564 (7734): 53–58. https://doi.org/10.1038/s41586-018-0712-z.

Cowton, Tom, Donald Slater, Andrew Sole, Dan Goldberg, and Peter Nienow. 2015. "Modeling the Impact of Glacial Runoff on Fjord Circulation and Submarine Melt Rate Using a New Subgrid-

Scale Parameterization for Glacial Plumes." *Journal of Geophysical Research: Oceans* 120 (2). https://doi.org/10.1002/2014JC010324.

Debreu, L., N. K.R. Kevlahan, and P. Marchesiello. 2020. "Brinkman Volume Penalization for Bathymetry in Three-Dimensional Ocean Models." *Ocean Modelling*. https://doi.org/10.1016/j.ocemod.2019.101530.

England, Mark R, Till J W Wagner, and Ian Eisenman. 2020. "Modeling the Breakup of Tabular Icebergs." *Science Advances* 6 (51): eabd1273. https://doi.org/10.1126/sciadv.abd1273.

Favier, L., N.C. Jourdain, A. Jenkins, N. Merino, G. Durand, O. Gagliardini, F. Gillet-Chaulet, and P. Mathiot. 2019. "Assessment of Sub-Shelf Melting Parameterisations Using the Ocean-Ice-Sheet Coupled Model NEMO(v3.6)-Elmer/Ice(v8.3)." *Geoscientific Model Development* 12 (6). https://doi.org/10.5194/gmd-12-2255-2019.

FitzMaurice, A., C. Cenedese, and F. Straneo. 2017. "Nonlinear Response of Iceberg Side Melting to Ocean Currents." *Geophysical Research Letters* 44 (11). https://doi.org/10.1002/2017GL073585.

Gladish, Carl V., David M. Holland, Aqqalu Rosing-Asvid, Jane W. Behrens, and Jesper Boje. 2015. "Oceanic Boundary Conditions for Jakobshavn Glacier. Part I: Variability and Renewal of Ilulissat Icefjord Waters, 2001–14." *Journal of Physical Oceanography* 45 (1): 3–32. https://doi.org/10.1175/JPO-D-14-0044.1.

Gladstone, Rupert M., Grant R. Bigg, and Keith W. Nicholls. 2001. "Iceberg Trajectory Modeling and Meltwater Injection in the Southern Ocean." *Journal of Geophysical Research: Oceans* 106 (C9): 19903–15. https://doi.org/10.1029/2000JC000347.

Goldberg, D. N., C. M. Little, O. V. Sergienko, A. Gnanadesikan, R. Hallberg, and M. Oppenheimer. 2012. "Investigation of Land Ice-Ocean Interaction with a Fully Coupled Ice-Ocean Model: 1. Model Description and Behavior." *Journal of Geophysical Research: Earth Surface* 117 (2): 1–16. https://doi.org/10.1029/2011JF002246.

Gwyther, David E., Benjamin K. Galton-Fenzi, Michael S. Dinniman, Jason L. Roberts, and John R. Hunter. 2015. "The Effect of Basal Friction on Melting and Freezing in Ice Shelf–Ocean Models." *Ocean Modelling* 95 (November). https://doi.org/10.1016/j.ocemod.2015.09.004.

Hausmann, U., J.-B. Sallée, N. C. Jourdain, P. Mathiot, C. Rousset, G. Madec, J. Deshayes, and T. Hattermann. 2020. "The Role of Tides in Ocean-Ice Shelf Interactions in the Southwestern Weddell Sea." *Journal of Geophysical Research: Oceans* 125 (6). https://doi.org/10.1029/2019JC015847.

Hopwood, M. J., D. Carroll, T. J. Browning, L. Meire, J. Mortensen, S. Krisch, and E. P. Achterberg. 2018. "Non-Linear Response of Summertime Marine Productivity to Increased Meltwater Discharge around Greenland." *Nature Communications* 9 (1): 3256. https://doi.org/10.1038/s41467-018-05488-8.

Huot, Pierre-Vincent, Thierry Fichefet, Nicolas C. Jourdain, Pierre Mathiot, Clément Rousset, Christoph Kittel, and Xavier Fettweis. 2021. "Influence of Ocean Tides and Ice Shelves on Ocean–Ice Interactions and Dense Shelf Water Formation in the D'Urville Sea, Antarctica." *Ocean Modelling* 162 (June): 101794. https://doi.org/10.1016/j.ocemod.2021.101794.

Jenkins, Adrian. 2011. "Convection-Driven Melting near the Grounding Lines of Ice Shelves and

Tidewater Glaciers.” *Journal of Physical Oceanography* 41 (12): 2279–94. https://doi.org/10.1175/JPO-D-11-03.1.

———. 2016. “A Simple Model of the Ice Shelf–Ocean Boundary Layer and Current.” *Journal of Physical Oceanography* 46 (6): 1785–1803. https://doi.org/10.1175/JPO-D-15-0194.1.

Jordan, James R., Paul R. Holland, Dan Goldberg, Kate Snow, Robert Arthern, Jean-Michel Campin, Patrick Heimbach, and Adrian Jenkins. 2018. “Ocean-Forced Ice-Shelf Thinning in a Synchronously Coupled Ice-Ocean Model.” *Journal of Geophysical Research: Oceans* 123 (2): 864–82. https://doi.org/10.1002/2017JC013251.

Jourdain, Nicolas C., Pierre Mathiot, Nacho Merino, Gaël Durand, Julien Le Sommer, Paul Spence, Pierre Dutrieux, and Gurvan Madec. 2017. “Ocean Circulation and Sea-Ice Thinning Induced by Melting Ice Shelves in the Amundsen Sea.” *Journal of Geophysical Research: Oceans* 122 (3): 2550–73. https://doi.org/10.1002/2016JC012509.

Lemieux, Jean-François, Frédéric Dupont, Philippe Blain, François Roy, Gregory C. Smith, and Gregory M. Flato. 2016. “Improving the Simulation of Landfast Ice by Combining Tensile Strength and a Parameterization for Grounded Ridges.” *Journal of Geophysical Research: Oceans* 121 (10): 7354–68. https://doi.org/10.1002/2016JC012006.

Lichey, Christoph, and Hartmut H. Hellmer. 2001. “Modeling Giant-Iceberg Drift under the Influence of Sea Ice in the Weddell Sea, Antarctica.” *Journal of Glaciology* 47 (158): 452–60. https://doi.org/10.3189/172756501781832133.

Marson, Juliana M., Paul G. Myers, Xianmin Hu, and Julien Le Sommer. 2018. “Using Vertically Integrated Ocean Fields to Characterize Greenland Icebergs’ Distribution and Lifetime.” *Geophysical Research Letters* 45 (9): 4208–17. https://doi.org/10.1029/2018GL077676.

Massom, R. A., P.T. Harris, Kelvin J. Michael, and M.J. Potter. 1998. “The Distribution and Formative Processes of Latent-Heat Polynyas in East Antarctica.” *Annals of Glaciology* 27 (January): 420–26. https://doi.org/10.3189/1998AoG27-1-420-426.

Massom, R. A., K. L. Hill, V. I. Lytle, A. P. Worby, M.J. Paget, and I. Allison. 2001. “Effects of Regional Fast-Ice and Iceberg Distributions on the Behaviour of the Mertz Glacier Polynya, East Antarctica.” *Annals of Glaciology* 33 (September). https://doi.org/10.3189/172756401781818518.

Nihashi, Sohey, and Kay I. Ohshima. 2015. “Circumpolar Mapping of Antarctic Coastal Polynyas and Landfast Sea Ice: Relationship and Variability.” *Journal of Climate* 28 (9): 3650–70. https://doi.org/10.1175/JCLI-D-14-00369.1.

Olason, Einar. 2016. “A Dynamical Model of Kara Sea Land-fast Ice.” *Journal of Geophysical Research: Oceans* 121 (5): 3141–58. https://doi.org/10.1002/2016JC011638.

Oppenheimer, M., et al. 2019. *Chapter 4: Sea Level Rise and Implications for Low Lying Islands, Coasts and Communities*. Edited by UK Cambridge University Press, Cambridge. IPCC speci. https://www.ipcc.ch/srocc/chapter/chapter-4-sea-level-rise-and-implications-for-low-lying-islands-coasts-and-communities/.

Partee, Sam, Matthew Ellis, Alessandro Rigazzi, Scott Bachma, Marques Gustavo, Shao Andrew, and Benjamin Robbins. n.d. “Using Machine Learning at Scale in HPC Simulations with SmartSim: An Application to Ocean Climate Modeling.” https://arxiv.org/pdf/2104.09355v1.pdf.

Pelletier, C, T Fichefet, H Goosse, K Haubner, S Helsen, P.-V. Huot, C Kittel, et al. 2021. "PARASO, a Circum-Antarctic Fully-Coupled Ice-Sheet - Ocean - Sea-Ice - Atmosphere - Land Model Involving f.ETISh1.7, NEMO3.6, LIM3.6, COSMO5.0 and CLM4.5." *Geoscientific Model Development Discussions* 2021: 1–59. https://doi.org/10.5194/gmd-2021-315.

Rackow, Thomas, Christine Wesche, Ralph Timmermann, Hartmut H. Hellmer, Stephan Juricke, and Thomas Jung. 2017. "A Simulation of Small to Giant Antarctic Iceberg Evolution: Differential Impact on Climatology Estimates." *Journal of Geophysical Research: Oceans* 122 (4): 3170–90. https://doi.org/10.1002/2016JC012513.

Rignot, E., Y. Xu, D. Menemenlis, J. Mouginot, B. Scheuchl, X. Li, M. Morlighem, et al. 2016. "Modeling of Ocean-Induced Ice Melt Rates of Five West Greenland Glaciers over the Past Two Decades." *Geophysical Research Letters* 43 (12): 6374–82. https://doi.org/10.1002/2016GL068784.

Schloesser, Fabian, Tobias Friedrich, Axel Timmermann, Robert M. DeConto, and David Pollard. 2019. "Antarctic Iceberg Impacts on Future Southern Hemisphere Climate." *Nature Climate Change* 9 (9): 672–77. https://doi.org/10.1038/s41558-019-0546-1.

Slater, Donald A., Dan N. Goldberg, Peter W. Nienow, and Tom R. Cowton. 2016. "Scalings for Submarine Melting at Tidewater Glaciers from Buoyant Plume Theory." *Journal of Physical Oceanography* 46 (6): 1839–55. https://doi.org/10.1175/JPO-D-15-0132.1.

Smith, Robin S., Pierre Mathiot, Antony Siahaan, Victoria Lee, Stephen L. Cornford, Jonathan M. Gregory, Antony J. Payne, et al. 2021a. "Coupling the U.K. Earth System Model to Dynamic Models of the Greenland and Antarctic Ice Sheets." *Journal of Advances in Modeling Earth Systems*, September. https://doi.org/10.1029/2021MS002520.

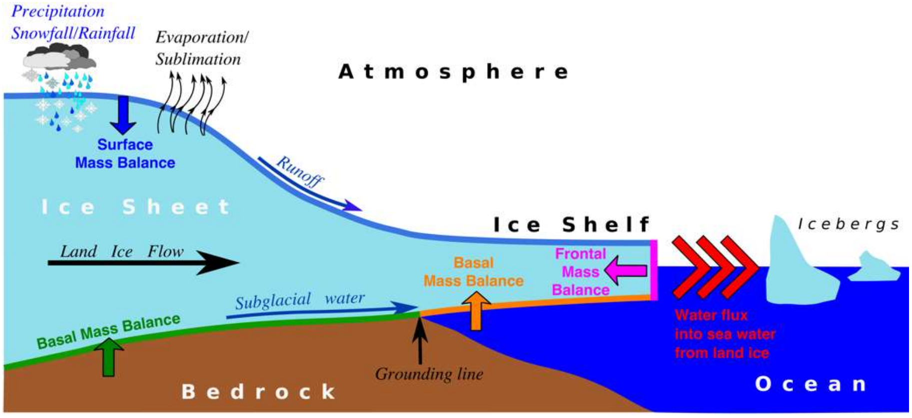
———. 2021b. "Coupling the U.K. Earth System Model to Dynamic Models of the Greenland and Antarctic Ice Sheets." *Journal of Advances in Modeling Earth Systems*, September. https://doi.org/10.1029/2021MS002520.

Stern, A. A., A. Adcroft, and O. Sergienko. 2016. "The Effects of Antarctic Iceberg Calving-Size Distribution in a Global Climate Model." *Journal of Geophysical Research: Oceans* 121 (8): 5773–88. https://doi.org/10.1002/2016JC011835.

Tournadre, J., N. Bouhier, F. Girard-Ardhuin, and F. Rémy. 2016. "Antarctic Icebergs Distributions 1992–2014." *Journal of Geophysical Research: Oceans* 121 (1): 327–49. https://doi.org/10.1002/2015JC011178.

Vaňková, Irena, and David M. Holland. 2017. "A Model of Icebergs and Sea Ice in a Joint Continuum Framework." *Journal of Geophysical Research: Oceans* 122 (11): 9110–25. https://doi.org/10.1002/2017JC013012.

Wei, Wei, Donald D. Blankenship, Jamin S. Greenbaum, Noel Gourmelen, Christine F. Dow, Thomas G. Richter, Chad A. Greene, et al. 2020. "Getz Ice Shelf Melt Enhanced by Freshwater Discharge from beneath the West Antarctic Ice Sheet." *The Cryosphere* 14 (4). https://doi.org/10.5194/tc-14-1399-2020.


Precipitation
Snowfall/Rainfall
Evaporation/
Sublimation
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Surface
Mass Balance
Runoff
Ice Sheet
Ice Shelf
Icebergs
Land Ice Flow
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Frontal
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Basal Mass Balance
Water flux
into sea water
from land ice
Grounding line
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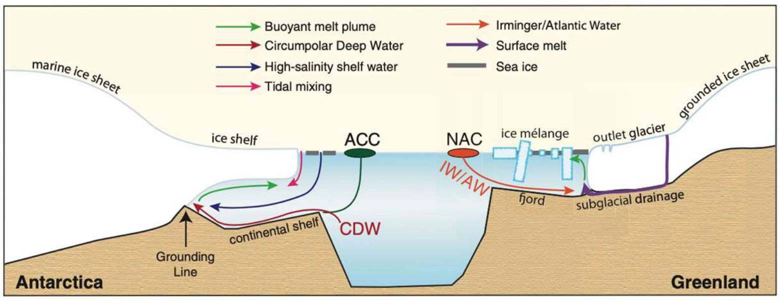
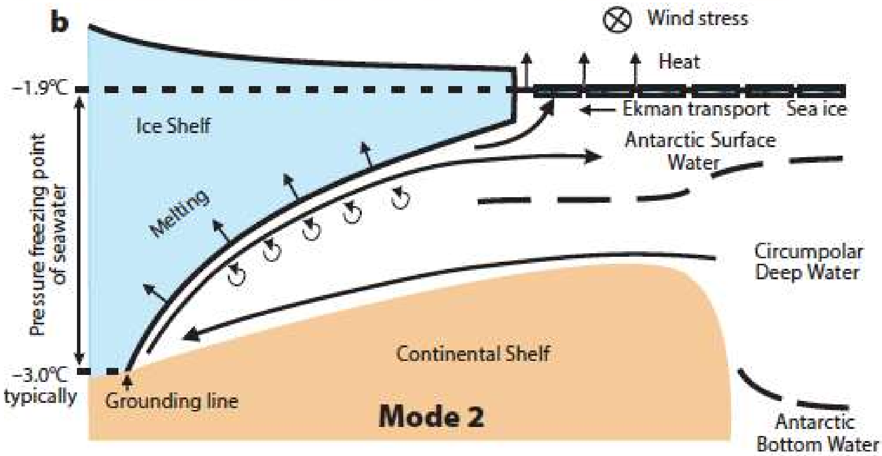

Buoyant melt plume
Circumpolar Deep Water
High-salinity shelf water
Tidal mixing
Irminger/Atlantic Water
Surface melt
Sea ice
marine ice sheet
grounded ice sheet
ice shelf
ACC
NAC
ice mélange
outlet glacier
IW/AW
fjord
subglacial drainage
continental shelf
CDW
Grounding
Line
Antarctica
Greenland


b
Wind stress
Heat
−1.9℃
Ice Shelf
Ekman transport
Sea ice
Antarctic Surface
Water
Pressure freezing point
of seawater
Melting
Circumpolar
Deep Water
Continental Shelf
−3.0℃
typically
Grounding line
Mode 2
Antarctic
Bottom Water

8 Tides

8.1 Introduction

In a numerical ocean model, tides are mostly a barotropic response to an astronomical forcing [and open boundary forcing if the domain is limited], with second-order impact on the general circulation and hydrography (via tidal mixing, tidal rectification and internal wave breaking). Tides were first introduced in NEMO 2.3 and then improved substantially in 3.6 with a better time-splitting scheme, the addition of astronomical tides, self-attraction-and-loading potential and better boundary conditions available in the module BDY.

The Tidal Working Group was formed in mid-2020 and started regular meetings in November 2020 with the aim of discussing current issues and suggesting potential improvements in NEMO. Below are a summary of the points that could be relevant to the NEMO strategy.

8.2 Data assimilation (or corrections methods)

OCGMs were not at their inception meant to resolve tides although with improved resolution they are now getting close to represent tides reasonable well in the deep ocean but with some difficulty in shelf areas and around Antarctica (where tidal resonance is an issue). To remedy the situation, some corrections are required and possible when an external source of data-assimilative tidal models is available (also referred as tidal “atlas”-es, i.e. FES or OSU). Two member groups have experimented with their own approaches, one consisting with spectrally nudging the tides in the momentum equations (https://www.sciencedirect.com/science/article/pii/S1463500321001463) and the second being a correction method re-injecting the unrepresented portion of the tides in a coarse OGCM. Both approaches offered promising results.

8.3 Internal wave drag parameterization

In order to represent the breaking of internal waves and release of the energy into mean potential energy, several groups tested different parametrizations and the discussion should continue and converge (gradH or U.gradH representation?).

8.4 Astronomical tidal potential and Self-Attraction and Loading (SAL)

Some improvements are possible in astronomical tides and SAL. One is to explore the use of the full astronomical potential (via only ephemeris; https://academic.oup.com/gji/article/168/3/999/2044447?login=true) instead of the more typical decomposition by tidal components. The SAL was initially given crudely as an extra term in the SPG as (k-h) ʒ. Self-attraction (k) is a positive feedback effect but loading (h) of the water column on the earth crust is a negative one) but given the existence of quite accurate tidal atlases, the SAL can in fact be diagnosed from them as a decomposition for each tidal constituent of spatially varying amplitude and phase, which can then be re-injected in the SPG. Another discussion was about taking into account the mean (or instantaneous) circulation contribution to SAL, via a user-defined spatially varying feedback coefficient (k-h) https://agupubs.onlinelibrary.wiley.com/doi/full/10.1029/2003JC002034.

8.5 Energetics

Normal mode decomposition is important to follow the energy flowing between the different dynamical components of the ocean. However, it was noted that an offline diagnostic was difficult. One suggestion is to either output the 3D fields at high frequency (including the pressure term which is not an option at this time) or doing the diagnostic online which implies relying on an additional library for the egeinvector decomposition. The latter would be also required if we follow the suggestion of Lemarié et al. (https://www.sciencedirect.com/science/article/pii/S0021999119305662)
which aims at better representing the barotropic mode in the mod-splitting technique.

8.6 Numerics

Numerical representation of the different contributions and interactions of tides with the rest of the dynamics is a field overlapping with other WGs but we think important to list of few items worth pursuing in the future:

- Vertical coordinate and related numerics (PG, accuracy order… etc)
- Baroclinic/barotropic interactions during time-splitting
- Varying bottom roughness (why having one value for the whole ocean when the morphology of the sea bottom is known to vary?)
- NH, WAD in very high resolution configurations

9 Marine Biogeochemistry and TOP Interface

Authors: T. Lovato, O. Aumont, G. Lessin

Marine biogeochemistry within the NEMO framework is addressed through a built-in biogeochemical component (PISCES, Aumont et al., 2015) and the TOP (Tracers in the Ocean Paradigm) module that provides a seamless, hardwired coupling interface with non-legacy marine ecosystem models such as MEDUSA (Yool et al., 2013), BFM (Lovato et al., 2020), ERSEM (Skakala et al., 2020) and BAHMBI (Palazov et al., 2021).
In this chapter, the foreseen evolution of NEMO components dealing directly and indirectly with marine biogeochemistry are outlined by considering the need to sustain the orthogonality between physical processes and oceanic tracers' dynamics (8.1), to extend the TOP workflow consolidated in previous years (8.2), and to foster the code readiness to handle future evolutions in marine biogeochemical models (8.3). These three main themes will be coordinated by the TOP working group representative and discussed/developed along with external experts from the European marine ecosystem modelling community.
As the NEMO modelling system is a multifarious space, additional emerging issues relating marine biogeochemistry and the different components of the framework are detailed within specific chapters. Here, only highlights of key cross chapter synergies will be provided to trace their relation with the main development themes of marine biogeochemistry and TOP interface.

9.1 Orthogonality between physical and biogeochemical components

Physical processes represent an essential driver in shaping the spatio-temporal distribution of living and non-living oceanic properties and the improvement toward both more accurate and up-to-date representation will benefit the simulation of marine biogeochemistry.
The following processes are foreseen to enable for major orthogonality between physical and biogeochemical components:

a. Enhance **particle dynamics in the water column** by allowing the selection of numerical schemes for vertical sinking with an increasing degree of accuracy (e.g. by using a technical design similar to the physical advection). A certain degree of flexibility is highly desirable within the modelling system to enable the balance between computational costs and accuracy (see e.g., Aumont et al., 2015). Moreover, this physical process directly applies to a variety of marine 'particles', like planktonic organisms and particulate organic/inorganic matter.
b. Improve **optical properties in the water column** by considering the potential contribution of remote sensing data in providing new insights on the role of coloured dissolved substances and particles. This will involve the revision of current schemes to ingest more complex definitions of the light spectrum and it will provide a more articulated representation of coastal zone dynamics (e.g. for CMEMS end-users).
c. Complement **seawater temperature and salinity definition** obtained from the two main formulations of the equation of state in NEMO: EOS80 provides the potential temperature and practical salinity, and TEOS10 the conservative temperature and absolute salinity. As a wide number of biogeochemical parametrizations derive from

experimental evidence, it would be useful to extend the biogeochemistry interface with at least the use of in-situ temperature fields. Further enhancements suggested as ‘best practices’ in Orr and Epitalon (2015) and recent literature should also be considered.

Synergy with **Chapter 11 - HPC**
A close collaboration with the HPC working group will be necessary to achieve a more effective and less computationally expensive solution to speed up marine quantities transport, namely by improving the numerical performance of advection and diffusion schemes inherited from the physical core.

9.2 Extend and consolidate TOP workflow

The TOP interface was soundly revised in the previous five years of development, such that the workflow modularity was largely consolidated and a number of handlers were created to advance in the integration with non-legacy biogeochemical models.
The following issues should be tackled to maintain the TOP workflow and further expand it:

a. **Interface technical developments** will be carefully evaluated to ensure a contained maintenance for the coupling of built-in and non-legacy biogeochemical models over the long term. However, new elements are still needed to further increase the interface modularity, such as the user-defined handling of restarts and outputs (namely in MY_TRC sub-module) and the possibility to use also three-dimensional forcing, e.g., to reproduce the release of tracer quantities within the model domain beyond the system boundaries.
b. **TOP workflow resilience** will benefit from the setup of a dedicated test case to verify the consistency of all data handlers and processes inherited from the NEMO core. This test case will likely be a new idealized configuration to evaluate the correct simulation of passive tracers’ dynamics due to physical schemes and prescribed surface, coastal, and lateral boundary conditions. In addition, this simplified configuration will provide a useful example of the generalized coupling interface to new users.

Synergy with **Chapter 13 - Verification and Validation**
The foreseen development of a dedicated TOP test case overlaps with the main activities of the V&V working group and it represents a useful interaction to increase the reliability of the code and support its long-term robustness.

9.3 Readiness for future biogeochemical complexity

The overall structure of the TOP interface is founded on the support of the marine pelagic component (arrays for state variables, time integration, etc.) and only a few elements are available to handle additional dynamical components. Nowadays biogeochemical models are increasingly addressing ecological processes occurring in other marine compartments (see e.g., Vancoppenolle & Tedesco, 2017; Lessin et al., 2018) and the following actions should be taken in the medium term:

a. **Infrastructure for marine sea-ice and benthic components** has to be designed in a more generalized, compatible framework as the existing one for the pelagic compartment. These elements should be integrated within the TOP interface to enable a coherent structure of the coupling framework, by designing dedicated sub-modules to provide access for shared memory arrays, initial and boundary conditions, and data saving. In addition, relevant physical processes should be inherited from the general NEMO framework (e.g. from SI3) and passed to the sub-module(s).
b. **Interfaces at the boundaries with the pelagic compartment** need to be included in the development of the new dynamical components. This would translate into the identification of suitable parameterizations and schemes to resolve the exchanges of biogeochemical quantities (e.g. inorganic nutrients, organic matter) at the seaice- and benthic-pelagic interfaces.

Synergy with **Chapter 6 - SEA-ICE**
The proposed development of a specific TOP interface to handle biogeochemical quantities within the marine sea-ice would benefit from the interaction with the SEA-ICE working group not only to design the interface, but also to identify key physical processes interacting with the sympagic ecosystem.

9.4 References

Aumont, O., Éthé, C., Tagliabue, A., Bopp, L., & Gehlen, M. (2015). PISCES-v2: an ocean biogeochemical model for carbon and ecosystem studies. Geoscientific Model Development, 8(8), 2465-2513.

Lessin, G., Artioli, Y., Almroth-Rosell, E., Blackford, J. C., Dale, A. W., Glud, R. N., ... & Yakushev, E. (2018). Modelling marine sediment biogeochemistry: Current knowledge gaps, challenges, and some methodological advice for advancement. Frontiers in Marine Science, 5, 19.

Lovato T., Vichi M., Butenschön M. (2020). Coupling BFM with Ocean models: the NEMO model V3.6 (Nucleus for the European Modelling of the Ocean). BFM Report series N. 2, Release 1.1, June 2020, Bologna, Italy, http://bfm-community.eu, pp. 31

Orr, J. C., & Epitalon, J. M. (2015). Improved routines to model the ocean carbonate system: mocsy 2.0. Geoscientific Model Development, 8(3), 485-499.

Palazov, A., Ciliberti, S. A., Lecci, R., Gregoire, M., Staneva, J., Peneva, E., ... & Agostini, P. (2021, April). The BS-MFC service and system evolutions within Copernicus Marine Service. In EGU General Assembly Conference Abstracts (pp. EGU21-5435).

Skakala, J., Bruggeman, J., Brewin, R. J., Ford, D. A., & Ciavatta, S. (2020). Improved representation of underwater light field and its impact on ecosystem dynamics: A study in the North Sea. Journal of Geophysical Research: Oceans, 125(7), e2020JC016122.

Vancoppenolle, M., and Tedesco, L. (2017). Numerical Models of Sea Ice Biogeochemistry. Hoboken, NJ: John Wiley & Sons, 492–515. doi: 10.1002/9781118778371.ch20

Yool, A., Popova, E. E., & Anderson, T. R. (2013). MEDUSA-2.0: an intermediate complexity biogeochemical model of the marine carbon cycle for climate change and ocean acidification studies. Geoscientific Model Development, 6(5), 1767-1811.

11 Two-way nesting capability (AGRIF)

WGLs: Jerome Chanut and Sebastien Masson

11.1 Weaknesses in the present implementation

11.1.1 External mode coupling

Dealing with the external mode is certainly the most difficult part to obtain a truly robust multi-grid mesh coupling. In the case of an implicit treatment of the free surface, *Haley and Lermusiaux (2010)* report various strategies, the best one leading to a tight and complex space-time implicit coupling. In the case of a split-explicit free surface as in NEMO, the external mode being sub-stepped for each baroclinic step, the question arises whether data exchange between grids should occur at barotropic or baroclinic level. The second option has been chosen in NEMO and initially in ROMS-AGRIF (*Penven et al, 2006*). This is mainly because it does not require a deep reengineering of the model flowchart. It does however lead to possibly growing errors at the grid interface, because of diverging barotropic mode solutions within their sub-integrations. Using radiative or Flather type in place of clamped open boundary schemes (*Penven et al. 2006*; *Herzfeld and Rizwi, 2019*) can help minimizing the mismatch, but at the expense of moving away an exact volume conservation.

Exchanging data at barotropic level makes the grid coupling entirely confined in space to what the numerical schemes require (e.g. 2 ghost points for at most 4th order schemes in NEMO). Controlling numerical noise near the interface can then be achieved thanks to a standard nudging technique. We point out that using time averaging of barotropic variables as done in most split explicit free surface models (at least in MOM5, ROMS and NEMO models) does however require extended time integration windows, which makes things slightly more complicated. Still, as described by *Debreu et al (2012)*, this is possible, at the expense of added complexity. We note that recent progress in understanding leading mode splitting errors (*Demange et al 2019*) has led to the design of barotropic time stepping schemes with ad-hoc built-in dissipation (dissipative barotropic time stepping is already an option in NEMO 4_2). This suppresses the need for time averaging, hence makes external mode exchanges even more simple.

The other advantage of sub-step exchange, is that it makes possible exact coupling with adjacent grids having the same refinement ratio. Hence, it opens up possibilities to truly multigrid nesting. The last subtle benefit is that the overlapping region can be removed from the parent domain, hence saving some computational time. This gain may however be compensated by the over cost of frequent grid exchanges. Generally speaking, the question of the actual cost of AGRIF procedures in a massively parallel context has to be addressed (see below).

11.1.2 Inter-grid connections

Data exchange for each nested grid is currently restricted to a single parent grid. This precludes from having, at least, “neighboring” grids, hence exchanges between grids having the same refinement level (e.g. the same horizontal resolution). Implementing neighboring grid connections would greatly help to rationalize areas targeted for refinement, allowing for instance, to follow complex coastlines (see *Holt et al, 2017*) or dynamically active regions (*Sein et al, 2016*). We stress that this feature requires, as a prerequisite, sub-step exchanges.

11.1.3 Conservation properties

In a finite volume context, as long as fluxes are exchanged between nested components, maintaining conservation relies on using conservative prolongation and restriction operators, both in space and time. Prolongation operators used in the space domain in NEMO are at least of 2nd order accuracy and basically the same as in *Debreu et al (2012)*. These ensure conservation of fluxes along cell faces. Restriction operators, which are very much similar to the “coarsening schemes” used to speed up BGC modelling (see below and *Bricaud et al, 2020*), garanty the conservation of divergence, tracer content and volume. In the end, conservation issues in NEMO, as in many other models, mainly come from the time dimension.

Volume is in any case perfectly conserved in the present implementation, taking advantage of the forward nature of the barotropic model between two consecutive baroclinic steps. This is nevertheless not the case for tracers, for which the model advection and diffusion schemes compute their own set of fluxes at the grids interface from exchanged tracer values (this still guarantees monotonicity if required). With time refinement, the LFRA time stepping (Leapfrog + Robert Asselin filtering) greatly complexifies the exchange of time-integrated fluxes over the right time interval which in addition precludes the conservation of internal momentum fluxes. Using “refluxing” methods as in *Debreu et al (2012)* can be envisioned, as a posteriori correction, but this is again impractical in a LFRA environment (*Herrnstein, 2015*). Ensuring perfect conservation should be re-considered in the upcoming, two-time level, RK3 framework.

11.1.4 Preprocessing stage

Online grid exchanges rely on the consistency of grids near the dynamical interface and to a lesser extent in the overlapping area. As a matter of fact, success of the grid nesting procedure greatly depends on what is done during the preprocessing of the mesh.

The mesh preprocessing for the whole nested grid hierarchy is now achieved, once in a row, thanks to the DOMAINcfg tool. It is highly recommended to maintain it in accordance with any new development of the nesting scheme. Ideally, to minimize inconsistencies, modules used in NEMO should be shared with the tool as much as possible.

Volume matching mostly relies on a crude 1st order topography matching. While it is a bit uncertain at this stage how Brinkman penalization[1] (Debreu et al. 2020) would fit into that paradigm, we suggest investigating its adaptation for a more “continuous” grid connection.

11.1.5 Documentation

NEMO AGRIF still lacks documentation of the nesting procedure itself. In particular, subtleties on the external mode coupling in a LFRA context, not explained elsewhere, need to be described precisely. A user guide describing how to set up a hierarchy of nested grids is needed too.

11.1.6 Other issues

- Missing functionalities with AGRIF (e.g. BDY, ice cavities, wetting and drying,...)
- Lumping AGRIF into BDY modules ?
- Remaining issues with the code converter (“target” attributes but not only).
- Use of AGRIF lexical converter for other purposes (mixed precision) ?
- Inconsistency between TKE/GLS time stepping and main time stepping (pronostic turbulence quantities lag by 1 baroclinic time step in the past) makes the implementation of two-way nesting impractical.
- Nesting and multistage RK3
- Nesting and ALE coordinates

[1] Brinkman’s penalization introduces concepts of porosity and permeability in the dynamical equations. Deviations from a smooth topographic enveloppe can then be easily represented though these new terms. This is currently under testing in NEMO (Madec, personal communication).

11.2 Use of AGRIF as an online coarsening tool

Coarsening physical variables to run a BGC model is now a current practice with NEMO (*Berthet et al, 2019*; *Bricaud et al, 2020*). Assuming that much of the relevant physical signal is above the grid effective resolution, it indeed greatly speeds up the modelling of tens of tracer variables. Technically speaking, the coarsening process is based on fluxes and divergence conservation principles that are actually identical to the ones used in the nesting restriction step.

Based on that redundancy, it seems natural to envision AGRIF as an online coarsening tool. The existing one is indeed not maintained anymore in versions 4 and later, and has some limitations: it has a fixed coarsening factor of 3 and does not deal with time refinement. Moreover, it relies on basic restrictions operators that could be advantageously replaced by higher order, more selective schemes, already shipped with the AGRIF library (see *Debreu et al., 2012*). The recent adaptation of the code to deal with global cyclic child grids[2] should make this adaptation even more straightforward.

11.3 Performances

Contrary to scientific production using AGRIF, up to now, there were little efforts really dedicated to the HPC aspects of AGRIF. AGRIF is often proposed as a solution for future configurations allowing to reach, at lower cost, very high resolution (km-scale) in places where it is needed. The viability of such a solution requires good HPC performances of AGRIF that must therefore be investigated and optimized. The library is parallelized with MPI and recent developments will offer some possibilities to run in parallel multiple zooms but a quantitative and extensive study of the HPC performances and the scalability of AGRIF in real applications have never been really explored. The 2-way nesting strategy implies interpolations between child and parent grids, which intrinsically generates communications that could slowdown simulations and limit the model scalability.

We first need to establish a comprehensive profiling of AGRIF zooms in NEMO simulations to quantify the impact of the library on NEMO HPC performances, to identify the HPC bottlenecks and propose solutions to suppress them including the potential use of GPU. This technical optimization must also be completed by a work on the numerical properties of AGRIF. In short, what is the HPC cost of the perfect conservation properties of AGRIF? Can we find better numerical schemes that cost less? Could we consider, at least for some applications, to downgrade the numerical properties of AGRIF if this allows us to significantly improve its HPC performances?

11.4 References

Berthet, S., R. Séférian, C. Bricaud, M. Chevallier, A. Voldoire and C. Ethé (2019): Evaluation of an Online Grid-Coarsening Algorithm in a Global Eddy-Admitting Ocean Biogeochemical Model. Journal of Advances in Modeling Earth systems. 11-6, 1759-1783.

Bricaud, C. J. Le Sommer, G. Madec, C. Calone, J. Deshayes, C. Ethe, J. Chanut, and M. Levy (2020): Multi-grid algorithm for passive tracer transport in the NEMO ocean circulation model: a case study with the NEMO OGCM (version 3.6). Geosci. Model Dev., 13, 5465–5483.

Debreu, L., N. Kevlahan, and P. Marchesiello (2020): Brinkman volume penalization for bathymetry in three-dimensional ocean models. Ocean Modelling, 145, 1-13.

[2] Global child grids could a priori have a North-fold T or F point pivot, hence odd or even coarsening factors. Existing coarsening assumes the same pivot on base and coarsened grids, hence only odd subsampling.

Debreu, L., Marchesiello, P., Penven, P. and G. Cambon (2012): Two-way nesting in split-explicit ocean models: Algorithms, implementation and validation. Ocean Modelling, 49-50, 1-21.

Demange, J., L. Debreu, P. Marchesiello, F. Lemarie, E. Blayo and C. Eldred (2019): Stability analysis of split-explicit free surface ocean models: implication of the depth-independent barotropic mode approximation. Journal of Computational Physics, 398, 108875.

Haley, P. J. and P. F. J. Lermusiaux (2010): Multiscale two-way embedding schemes for free-surface primitive equations in the "Multidisciplinary Simulation, Estimation and Assimilation System". Ocean Dynamics, 60, 1497-1537.

Herrnstein, A. R. (2005): A Parallel Ocean Model With Adaptive Mesh Refinement Capability for Global Ocean Prediction. Phd thesis, LLNL, 258p.

Herzfeld, l. and F. Rizwi (2019): A two-way nesting framework for ocean models. Environmental Modelling and Software 117, 200-213.

Holt, J., P. Hyder, M., Ashworth, J., Harle, H. T., Hewitt, H., Liu, A. L., New, S., Pickles, A., Porter, E., Popova, J. I., Allen, J., Siddorn, and R. Wood (2017): Prospects for improving the representation of coastal and shelf seas in global ocean models, Geosci. Model Dev., 10, 499–523.

Penven, P., L. Debreu, P. Marchesiello and J. C. McWilliams (2006): Evaluation and application of the ROMS 1-way embedding procedure to the central california upwelling system. Ocean Modelling, 12, 157-187.

Sein, D. V., S. Danilov, A. Biastoch, J. V. Durgadoo, D. Sidorenko, S. Harig and Q. Wang (2016): Designing variable ocean model resolution based on the observed ocean variability. Journal of Advances in Modeling Earth systems. 8, 904-916.

12 Adaptations for High Performance Computing

WGL: Italo Epicoco

12.1 Introduction

The chapter aims at defining the optimization strategy of the NEMO code in order to satisfy the scientific community requirements in terms of elapsed time needed to perform high-resolution and complex simulations. The strategy has to take into account the model development on one side and the features of new computing systems on the other one.

From the numerics point of view, in the last years NEMO community efforts focused on both the development of very high-res configuration (NEMO at 1/36°) and the definition of an efficient kernel reducing time step data dependency, that means reducing need to exchange data among parallel processes.

Similarly, HPC development strategy aimed at reducing communication frequency and elapsed time through a reengineering of the parallel algorithm and an innovative implementation of data exchanges. At the same time, this reengineering process allowed us to explore new memory access patterns and then to reduce the computing time on the single node. However, these strategies need to be consolidated and their exploitation will be extended in the future. Indeed, the implementation of this kind of optimizations requires the algorithm to be completely rethought where its nature seems to be sequential and represents a good starting point to explore new implementation strategies, such as the multicore parallelization, also considering the portability on heterogeneous systems.

The NEMO code performance is still limited by the memory-bandwidth; the optimization strategies should be directed towards the reduction of memory access i.e. by extending and consolidating the tiling approach and by reducing the temporary arrays. On the other hand, the new code development should be oriented towards the GPU-based architectures or vector processors.

Concerning this last point, the adoption of DSL as a tool for improving the automation and the abstraction of the implementation process from the system architecture is a viable solution to be evaluated.

As regards the use of mixed-precision in the NEMO code, the work done shows an improvement in terms of simulation time, but more investigation is needed to evaluate the impact on the results accuracy.

Finally, other parallelism levels can be exploited, i.e. parallelize the tracers computation or introduce functional parallelism on different model components.

12.2 Consolidating the current optimizations (Daley)

In the last three years many new features and transformations to the code have been introduced. Among the main transformations that have had an impact on the performances are the halo extension, the north fold optimization, the I/O optimization avoiding to save redundant data, the XIOS extension also for reading restart files and forcing files and the management of the calculation through tiles. Many of these optimizations have led to significant benefits, other optimizations seem not to be completed as they did not bring the benefits expected at the beginning. The use of tiling is one of them.

The NEMO version 4.2 candidate release allows the number of halo points in an MPI domain to be specified (the main choices being 1 or 2). When a 2-point halo is chosen the number of exchanges between halos is greatly reduced and a 2D horizontal tiling of the domain can be used for most 3D calculations. In practice on SIMD processors the first (ji) index cannot be tiled without degrading the model performance. The computational cost of some subroutines in some configurations (typically those with relatively low vertical resolution) is reduced by 30-50%. Somewhat larger and more consistent improvements in performance can be achieved for some subroutines by tiling the calculations also in the vertical direction. We intend to implement this for the most costly routines where we can.

The long term goal of the tiling is to allow OpenMP threads to perform the calculations for the tiles in parallel. During the initial serial implementation, it became clear that this was not easy to achieve due to overlap between tiles and "non-overlapping" DO loops were introduced in some subroutines to ensure correctness of the calculations. A new design is being sought for the tiling that will allow the tiles to be calculated independently (and hence be suitable for OpenMP) and that will not be difficult for code developers to understand. The design is likely to require adding an extra tile dimension to some (preferably a small number of) permanent arrays, similar to the approach used in the MITgcm implementation of tiling.

12.3 Multicore parallelisation

Tiling offers a natural way toward a multicore parallelization of NEMO, and OpenMP would represent a suitable solution to maintain single code with support for different architectures. However several key aspects of the model need to be significantly revised in order to support a full multicore parallelization. For example: the iceberg code is an inherently sequential algorithm that needs to be re-written; and as previously mentioned the current implementation of tiling needs revising to be suitable for OpenMP.

12.4 Moving towards DSL

Like all large models, the development of NEMO is continually striving to find the right balance between the three competing demands of Portability, Performance and Productivity (the so-called "Three P's"). Of these three, NEMO development has largely prioritised Portability and Productivity which makes sense because it is a large, rapidly-evolving code base developed and used by scientists at many different institutions. It has a well-optimised distributed-memory parallelisation which has served it well for many years and has no dependencies other than on the MPI library.

However, the need to ensure the Productivity of domain scientists, combined with the rapid evolution of different HPC programming models also means that NEMO is currently unable to take advantage of developments in hardware such as GPUs. At the moment this primarily impacts Performance since NEMO is unable to take advantage of the significantly-greater memory bandwidth provided by such devices. However, this adherence to a single programming model is also beginning to impact Portability: to illustrate this we note that six of the top-10 supercomputers in the Top500 List of June 2021 utilise GPUs to provide the vast majority of their computational power.

One approach to being able to develop a model that can satisfy all three of the 'P's is that of Domain-Specific Languages. Traditionally, this means that a domain scientist writes their model in a language specifically designed to be expressive and powerful for their particular field. This code is then processed with a domain-specific compiler that is able to generate performant code for a variety of hardware, utilising domain-specific knowledge to do so. The main advantages of this approach are in its "separation of concerns": domain scientists can concentrate on the scientific aspects of the code while computational scientists can optimise the code that is generated or target entirely new hardware by working on aspects of the compiler.

However, there are significant drawbacks to this approach, particularly for a large community model such as NEMO. The primary one is that the model must be completely re-written in the DSL which is a massively costly and time-consuming process that would effectively halt all scientific development while it was carried out. Not only that, all developers would have to be trained in the DSL. A further drawback relates to the underlying toolchain - a language is only useful so long as there is a reliable compiler that can generate code for the hardware that a scientist wants (or needs) to use. For these reasons, adopting a traditional DSL approach for a model like NEMO is simply untenable.

What is required is a way of evolving an existing code base such that it can take advantage of DSL technology without having to be re-written from scratch. This approach has been explored in the ISENES2, ESiWACE2 and ExCALIBUR Marine Systems Projects which have worked and are working to extend the 'PSyclone' code-generation and transformation system so that it is able to work with existing, unmodified NEMO source code. In a sense, this treats the NEMO code with its associated coding standards as a DSL and thus no (or only very minor) re-writing of the model is required: there is no need to switch from Fortran and thus, in the absence of PSyclone, the code remains as portable as it is today.

PSyclone is developed by STFC's Hartree Centre, the UK Met Office and the Australian Bureau of Meteorology. It forms a key part of the build system for the UK Met Office's new LFRic atmosphere model, due to go operational within the next two years. As such, the UK Met Office is committed to its ongoing development and support.

To date, the primary focus has been on enabling NEMO to make use of the performance benefits of GPU hardware: PSyclone has been extended and developed such that it is now able to process a complete NEMO configuration (based on the GO8 configuration from the Met Office) and transform it such that it can be run on GPU. When this is done, the ORCA1, ocean-only version of the configuration runs on a single NVIDIA V100 GPU at 2.3x the speed of a Skylake socket. Work has only just begun on looking at the SI^3 component, where acceleration is more challenging, but currently the whole configuration (including SI^3) runs some 30% faster than on a full Skylake socket.

The PSyclone-processed, ORCA12 configuration has been run on up to 192 GPUs on the JUWELS Booster and Marconi machines. However, performance is currently only equivalent to running on the same number of Intel Skylake sockets. The reason for this is that all halo exchanges are currently going via the host CPU instead of directly between GPUs. This is because PSyclone currently uses NVIDIA's managed memory technology to control data movement between host and GPU and it is not possible to use this in conjunction with NVIDIA's GPU Direct technology. Longer term it seems inevitable that this restriction will be lifted since it is currently a major limitation of managed memory. However, PSyclone is not constrained to relying upon managed memory and work is ongoing to extend its existing support for managing data movement explicitly.

All of this work is very promising but much remains to be done. Some of the remaining issues are:

1. Full integration of PSyclone processing into the build system and SETTE suite;
2. Testing with the latest version of NEMO;
3. Addressing those parts of the NEMO code base that do not work well on GPU (e.g. the Iceberg component, statement functions);
4. Testing with other components, especially AGRIF;
5. Extending and fixing known issues in PSyclone;

6. Extending PSyclone to target GPUs (such as those from AMD and Intel) using OpenMP rather than OpenACC;
7. Improving GPU performance (target of 3-4x a CPU socket).

If PSyclone is adopted as part of the NEMO build system then it opens the way for a wide range of hardware- and/or configuration-specific optimisations to be developed since these optimisations take the form of separate, Python transformation scripts instead of having to be hardcoded in Fortran. This is not only quicker to do (one script can be applied across the whole code base) but can be done independently of the ongoing scientific development of NEMO. It is therefore a very attractive prospect. Looking beyond GPUs, there are several performance and correctness aspects that PSyclone could help to address:

1. Optimisation of existing code base for current CPU architectures (e.g. loop fusion, elimination of array temporaries, etc.);
2. Identifying halo exchanges and validating their correctness;
    a. Making use of the extended halo-depth support to automatically use redundant computation to eliminate halo exchanges;
3. Transforming the code base for execution on other architectures (such as vector machines);
4. Addition of threading parallelisation using OpenMP;

PSyclone is also being extended to generate the adjoint of the tangent-linear form of LFRic. This functionality is being constructed such that it is general purpose and can, in principle, be applied to any tangent-linear code written in Fortran.

12.5 Mixed precision

During the last decades, the available computational performance has been steadily increasing (Moore's law), while the increase in CPU memory speed has been lagging. As a result, many computational codes, such as NEMO, have seen that CPU speed is no longer the main limiting factor for their performance, becoming memory-bound applications.

On the other hand, most modern processors implement vector operations, which allow doubling the number of floating-point operations per cycle by halving the size of the operands.

As a result, mixed-precision approaches emerge as a powerful solution to improve application efficiency by improving the speed at which variables are read from memory and increasing the degree of parallelism in a single core.

In the last few years, different works have applied precision reduction techniques to improve the performance of different codes, from the routine level to the whole application, including Earth Sciences codes. One clear example is the IFS model, whose code was migrated to mixed-precision so that most of the fields are represented in single precision and finally put in production in 2021.

Nevertheless, entirely moving a computational model to mixed-precision can be an arduous task. Unavoidably, a decrease in the precision used to represent the operands will lead to different results of the operations that they are involved, with a high probability of having numerical errors and instabilities, especially in computational models of a chaotic nature that perform a considerable number of operations at different scales and in which small perturbations can be propagated and amplified, leading to different process representations. As a result, one of the biggest challenges that this kind of work poses is identifying which variables can be safely demoted to an inferior representation, especially if the software is intended to provide results comparable to the higher precision counterpart.

These questions were very briefly exposed in the previous development strategy document, written at the moment when the NEMO community was starting to pay attention to this problem. Since then, the Barcelona Supercomputing Center (BSC) has been working on a methodology to move FORTRAN codes to mixed-precision in an automatic way, intending to simplify the most challenging steps of transferring a complete model to mixed-precision. Those involve identifying the variables that can safely move to an inferior precision and performing the necessary changes in the code to not affect the interoperability with other variables or operands represented at the same or another precision level.

The methodology has been materialized in a set of tools doing all the necessary analysis to classify the different fields into two groups (those whose precision can be reduced and those which need to preserve their current representation) to then create an actual implementation in the target precision.

Those analyses use a precision emulator and are based on a set of tests (variable, threshold pairs) to decide if they succeed or not. These variables are model diagnostics and internal fields whose value is obtained from actual model runs. As a result, the methodology is dependent on the model configuration used at the time to do the analysis.

Consequently, the BSC and the NEMO consortium agree that the accessibility to this set of tools is a key asset to promote the use of mixed-precision in NEMO.

On the other hand, having a minimum set of changes in NEMO like a core set of function interfaces for different precision will facilitate the operation of the automatic tool. A considerable part of those modifications were developed in collaboration with the ECMWF and are currently part of the NEMO trunk.

Likewise, the number of code changes to be done for a new configuration to run in lower precision can be smaller if there is already a reference configuration prepared to run in that precision. For that reason providing mixed-precision support for a configuration of the ORCA1 family will be beneficial in the long run, and the plan is to do it once that the automatic tool is prepared to be used by the consortium members.

12.6 Exploring further levels of parallelisation (Italo)

NEMO implements a single level of parallelism based on domain decomposition and the distribution of subdomains to MPI processes. However, other levels of parallelism based on functional decomposition could be explored, through the allocation of different tasks/components to the processes or threads.

A solution to be investigated could be to split the treatment of tracers, in particular when biogeochemistry is activated and the same operations must be performed on several tracers at each time step. A careful analysis of the code would allow to address some key issues such as the data dependency among tracers, the rethinking of the code to increase the size of the parallel region (loop on the tracers), the choice of the most suitable parallelization strategy, also taking into account the characteristics of the reference architecture.

There is therefore a close correlation between this activity and those above described in the chapter: the choice of the parallelization strategy depending on the target architecture could be automatically implemented by the DSL, perhaps favoring multicore parallelization solutions while the rethinking of the code could also favor tiling techniques.

13 Artificial Intelligence and Machine Learning

WGL: Julien Le Sommer, Nov. 2021

13.1 Context and purpose of this chapter

While advanced statistical methods and statistical learning have long been used in geosciences and remote sensing for solving inverse problems (Larry et al. 2016), we have witnessed over the past 5 years a very fast increase in the number of applications of *machine learning* (ML, see appendix), and specifically deep learning (DL, Goodfellow et al. 2016), to the field of fluid mechanics (Brunton est al. 2020) and computational fluid dynamics (Kochkov et al. 2021). This acceleration reflects a more general trend with a growing number of applications of ML to physical sciences (Carleo et al. 2019) and scientific computing.

Several new usages of machine learning relevant to the design and the usage of geoscientific models have emerged over this period, with published proof of concepts of applications for calibrating model parameters (Couvreux et al. 2021), for designing subgrid closures (Bolton and Zanna, 2019), for downscaling model data (Stengel et al. 2020), for accelerating the execution of specific code components (Chantry et al. 2021), for guiding the design of numerical schemes (Zhuang et al. 2021, Magiera et al. 2020), for learning underlying equations of motions (Champion et al. 2019), or for building representation of model errors (Bonavita and Laloyaux, 2020).

How (and how fast) ML will eventually affect the landscape of numerical tools used for studying and predicting oceanic flows and sea-ice dynamics is still unclear at this stage. Indeed many of the works cited above are still exploratory proof of concepts which do not exhibit yet the technological readiness for being implemented and maintained in production codes like NEMO. But the field is moving fast with many on-going research projects across the world. It is therefore reasonable to anticipate that the technological readiness of these applications will increase rapidly, and that new areas of applications could emerge over the period covered by this strategy (2023-2027).

We anticipate that, by 2027, physics-based models, as NEMO, will still be widely used and their structure will not be deeply affected by ML. Still, ML will probably by then often be used for analyzing their output and for calibrating their parameters. It is also likely that porting some specific code components to GPUs through emulation will be a mature and viable option. We also anticipate that ML will at that stage provide realistic opportunities for improving prediction systems involving data assimilation, and practical options to better exploit hybrid computer architectures. We also anticipate that ML will provide a framework for more systematically leverage observations in the design of the direct models used in prediction systems (Schneider et al. 2017).

In this context, the ambition of this chapter is to define some practical actions that can (i) foster the exploration of ML applications to the design and usage of the NEMO code and (ii) prepare NEMO development in this area beyond 2027. This chapter focuses on applications of ML only to the extent that they require specific developments into the NEMO code. For instance, implementing a subgrid closure or a numerical scheme designed with ML but expressed as a closed form equation (as the ones obtained with equation discovery approaches, see e.g. Zanna and Bolton 2020), would not require major changes to the NEMO code. Similarly, using ML-based approaches for calibrating model parameters would not a priori require any change of the NEMO code itself. On the contrary, implementing and maintaining subgrid closures expressed as NN may require a dedicated interface and should therefore be discussed in this document.

13.2 Key areas of applications of ML relevant to the development of NEMO

13.2.1 Better accounting for unresolved scales with ML

The use of ML for designing subgrid closures, and more generally improving the representation of unresolved scales and processes, has attracted quite some attention over recent years in the geoscientific and climate modelling community. Published works relevant to ocean model development have mostly focused on the representation of ocean macro-turbulence (see Zanna and Bolton 2021 for a recent review of mesoscales eddy closures with ML) but applications can be thought of for many different processes and scales. Given the (relative) maturity of the reflections in the computational fluid mechanics community on these questions, the design of subgrid closures appears as a reasonably low hanging fruit for applying ML to ocean model design. It should be noted though that, at the time of writing, the most advanced *interactive* ocean simulations with ML are still based on idealized flow configurations (as for instance Bolton and Zanna 2019, Guillaumin and Zanna 2021), while realistic ocean simulations have only been used for *non-interactive* inference so far (Partee et al. 2021), but this limitation should most likely soon be overcome. Current challenges are associated with how to account for the different flow regimes encountered at different locations across ocean basins, how to optimally define the filtering operator used to formulate the ML problem, how to bring prior physical or mathematical knowledge in the learning process (Frezat et al. 2021) and how to combine deterministic and stochastic components of eddy closures. Besides the representation of ocean macro-turbulence, ML could also probably be used for improving the representation of vertical physics in the OSBL, of fine scale processes at the air-sea interface, and of unresolved processes at the ice-sheet/ocean interface. All these examples would a priori use information drawn from finer resolution models (possibly down to LES simulations). Depending on the specific problem, the *technology readiness level* of applications of ML to represent unresolved scales range from intermediate to high.

13.2.2 A high potential emerging methodology : deep emulation

Deep emulation is another important area of application of machine learning relevant to ocean/sea-ice models development that has emerged over recent years. *Emulators* (aka *surrogate* models) are statistical models that learn to mimic the behavior of pre-existing numerical codes at reduced numerical cost. Emulators are used quite extensively for sensitivity analysis or for calibrating model parameters (see for instance Salter and Williamson, 2016, Williamson et al. 2017). In this context, emulators are generally aiming at reproducing some summary statistics of model trajectories (as for instance spatially and temporally averaged temperature bias). More recently, thanks to the versatility of deep neural networks as general purpose approximators, machines have been trained to emulate not only summary statistics of model trajectories but the entire time evolution of the full model state along model trajectories (Nonnenmacher & Greenberg, 2021; Kasim et al. 2020). Such *deep emulators* have successfully been used for reducing the cost of existing parameterization in atmospheric models and porting specific code components to GPUs (Chantry et al. 2021). Moreover, because automatic differentiation is readily available in ML libraries, deep emulation can also be used as a strategy for approximating the linear tangent and adjoint operators of model components or entire models (Hatfield et al. 2021)[3]. Deep emulation could therefore eventually open the possibility to formulate inverse problems for adjusting specific model parameters or for guiding the development of new code components with observations (Schneider et al. 2017), while allowing more versatility to better exploit future computing architectures. In this sense, deep emulation could

[3] It should be noted that we are here referring to an adjoint operator describing not only the sensitivity of model solutions to the model state but also to model parameters (as opposed to what was previously available with NEMO-TAM).

offer an alternative route to a full rewriting of our models in differentiable frameworks (see appendix) as undertaken for instance by the CliMA consortium. The *technology readiness level* of deep emulation ranges from low (approximation of the adjoint operator of the full code) to intermediate (porting specific code components to GPU).

13.3 Analysis of the need and propositions for NEMO

13.3.1 Practical tasks involved for using ML into NEMO

In practice, ML models should be trained (*learning* step) before being used (*inference* step). Most applications of ML to geoscientific models so far : supervised learning from datasets of model output, few applications of inference at the runtime (none with ocean models beside Partee et al. 2021)

In terms of tasks at the runtime in a NEMO application, three very different tasks are:

- *Interactive inference* : call a pre-trained ML model and modify the NEMO model state based on the output of the ML model (ML model can be run on GPU or CPU with good performance)
- *Online learning* : optimizing parameters of a ML model with a training objective based on the NEMO model state as a single simulation is progressing (ML model should be trained on GPU)
- *Interactive learning* : optimizing the parameters of a ML model with a training objective which evaluation requires to call specific components of the NEMO code independently or to run several NEMO simulations (ML model should be trained on GPU)

13.3.2 Overall ambition

(i) Allow for easy implementation of pre-trained closures into NEMO (interactive inference)

(ii) Make it simple to maintain a code component encoded as a NN into NEMO

(iii) Make it simple to use NEMO for testing new ideas in projects; making it a tool of choice for the research community

13.3.3 The question of the interface

A key question is to define how ML models can be encoded and maintained into NEMO for *interactive inference*. Several options, each coming with pros/cons :

- (a) Implement NN in FORTRAN (as for instance Curcic et al. 2019). But : Does not allow for online learning, difficult to maintain.
- (b) An interface to a specific ML library, as for instance FORTRAN-Keras Bridge (Ott et al. 2020). But : Not clear which framework to invest on in fast moving technological landscape.
- (c) A more generic interface (ML framework agnostic). several existing options inc. SmartSim (see appendix below), Melissa (developed by INRIA/DataMove).

We think that we should adopt option c, because :

- ML is a fast moving field and we should not be attached to a specific library as the technological landscape may evolve very fast;
- this would allow to optimize the orchestration of the inference on multiple processors more easily;
- this would allow for testing online learning (short term), and prepare interactive learning (mid term), therefore opening the possibility to investigate the design of deep emulators.

13.3.4 Practical propositions :

[An unconsolidated list of propositions at this stage]

- Define a robust procedure to interface NEMO with ML libraries (possibly with SmartSim) and its articulation with XIOS
- Define a procedure for storing/sharing pre-trained ML models with NEMO codebase.
- Develop, implement and maintain a subgrid closure encoded as a NN (to be defined in collaboration with other NEMO WGs)
- Establish collaborations on questions related to the orchestration of online learning and deep emulation (eg with ECMWF, INRIA/DataMove)
- Establish long term collaborations with super-computer vendors (eg. HPE, Bull, NVidia) on question related to ML libraries/ performance, in connection with HPC WG
- Improve the modularity of NEMO code components in order to prepare the emulation of code components beyond 2027
- Propose dedicated training on ML and ML/HPC to NEMO ST members
- Investigate which part of the NEMO could be accelerated and ported to GPU through emulation (e.g. sea-ice rheology ? NEMO-ICB module ?)
- Establish strong collaboration on ML-related matters with the DA WG, in order to investigate : (i) whether emulation could be an option for developing NEMO linear tangent (ii) how ML could be leveraged for estimating more systematically model parameters through ensemble simulations

13.4 Appendices :

13.4.1 Machine Learning

Machine learning (ML) is a vast field, which entails a large range of methods and algorithms for building numerical codes that learn how to accomplish their tasks. The behavior of the resulting numerical codes is therefore not prescribed a priori, but rather depends on parameters that should be learned in order for the numerical code to meet a prescribed objective. ML algorithms can be leveraged for different sorts of tasks as for instance : clustering, dimensionality reduction, classification or regression problems. ML entails a vast zoo of methods which differ in speed and accuracy. A key dimension of the modern ML landscape is that ML algorithms are encoded in ML libraries as for instance PyTorch, TensorFlow, Scikit-learn, which allows to easily combine and reuse pre-existing building blocks for solving new problems.

13.4.2 Neural networks

A neural network (NN) is a specific type of machine consisting in a series of mathematical operators (called “layers”) which parameters can be trained in order to meet a prescribed training objective.

Each layer combines an affine transformation (defined by its weights and biases as parameters) and a nonlinear operator (called activation). This structure implies that all the layers are piecewise differentiable. One can therefore compute analytically the derivative of the training objective with respect to the network parameters (weights and biases). Neural networks are generally encoded in dedicated software packages (eg. PyTorch, TensorFlow). The automatic differentiation and the gradient descent algorithms available in these packages allow optimizing the NN parameters on any training objective.

13.4.3 Differentiable programming

An emerging field at the interface between scientific computing and machine learning. Can be seen as a generalisation of Physics Informed deep learning. Not only data but also prior physical laws and applied math knowledge (eg. numerical schemes). Made possible because of the advances in automatic differentiation and DL frameworks. Allow to learn any aspects/component of a code. Often learns with less data. Mention Julia/JuliaDiff/Flux ecosystem, Jax/Flax. In our field, mention oceananigans.jl and the CliMa consortium (...).

13.4.4 The SmartSim library

This open-source library developed by HPE/Cray-lab is one of the several available software options for interfacing pre-existing scientific codes with ML libraries (e.g. TensorFlow or PyTorch). SmartSim (https://github.com/CrayLabs/SmartSim) is specifically aiming at providing a lightweight, non-intrusive and efficient interface for C, C++ or FORTRAN simulators using MPI. SmartSim relies on an in-memory data structure store (Redis) which allows diskless IOs. SmartSim has been used with the MOM6 ocean model for online inference (Partee et al. 2021). This library could also be used for orchestrating the production of (interactive) ensemble simulations or for outsourcing computations on GPUs (e.g. diagnostics). Some overlap with Melissa developed by INRIA (https://gitlab.inria.fr/melissa).

13.4.5 On-going ML related activities in NEMO ecosystem

We here provides an *unconsolidated* list of on-going or planned activities that could have direct implications on the NEMO code by 2027 :

- Representation of fine scale air-sea interactions (F. Lemarié, INRIA, Grenoble, in connection with the CROCO group)
- Closures for submesoscales (J. Le Sommer, IGE, Grenoble, as part of the M2LINES project)
- Coupling interface between ice sheet models and coarse resolution ocean model (N. Jourdain, IGE, Grenoble)
- Surface wave model emulation (Oxford, ECMWF)
- [list to be completed]

13.5 References

Bolton, T., & Zanna, L. (2019). Applications of Deep Learning to Ocean Data Inference and Subgrid Parameterization. In Journal of Advances in Modeling Earth Systems (Vol. 11, Issue 1, pp. 376–399). American Geophysical Union (AGU). https://doi.org/10.1029/2018ms001472

Bonavita, M., & Laloyaux, P. (2020). Machine Learning for Model Error Inference and Correction. Wiley. https://doi.org/10.1002/essoar.10503695.1

Brunton, S. L., Noack, B. R., & Koumoutsakos, P. (2020). Machine Learning for Fluid Mechanics. In Annual Review of Fluid Mechanics (Vol. 52, Issue 1, pp. 477–508). Annual Reviews. https://doi.org/10.1146/annurev-fluid-010719-060214

Carleo, G., Cirac, I., Cranmer, K., Daudet, L., Schuld, M., Tishby, N., Vogt-Maranto, L., & Zdeborová, L. (2019). Machine learning and the physical sciences. Reviews of Modern Physics, 91(4), 045002. https://doi.org/10.1103/RevModPhys.91.045002

Champion, K., Lusch, B., Kutz, J. N., & Brunton, S. L. (2019). Data-driven discovery of coordinates and governing equations. In Proceedings of the National Academy of Sciences (Vol. 116, Issue 45, pp. 22445–22451). Proceedings of the National Academy of Sciences. https://doi.org/10.1073/pnas.1906995116

Chantry, M., Hatfield, S., Dueben, P., Polichtchouk, I., & Palmer, T. (2021). Machine learning emulation of gravity wave drag in numerical weather forecasting. Journal of Advances in Modeling Earth Systems, 13(7). https://doi.org/10.1029/2021MS002477

Couvreux, F., Hourdin, F., Williamson, D., Roehrig, R., Volodina, V., Villefranque, N., Rio, C., Audouin, O., Salter, J., Bazile, E., Brient, F., Favot, F., Honnert, R., Lefebvre, M., Madeleine, J., Rodier, Q., & Xu, W. (2021). Process-Based Climate Model Development Harnessing Machine Learning: I. A Calibration Tool for Parameterization Improvement. In Journal of Advances in Modeling Earth Systems (Vol. 13, Issue 3). American Geophysical Union (AGU). https://doi.org/10.1029/2020ms002217

Curcic, M. (2019). A parallel Fortran framework for neural networks and deep learning. ArXiv:1902.06714 [Cs, Stat]. http://arxiv.org/abs/1902.06714

Frezat, H., Balarac, G., Le Sommer, J., Fablet, R., & Lguensat, R. (2021). Physical invariance in neural networks for subgrid-scale scalar flux modeling. *Physical Review Fluids*, *6*(2), 024607. https://doi.org/10.1103/PhysRevFluids.6.024607

Goodfellow, I., Bengio, Y., & Courville, A. (2016). Deep learning. The MIT Press.

Guillaumin, A. P., & Zanna, L. (2021). Stochastic-deep learning parameterization of ocean momentum forcing. Journal of Advances in Modeling Earth Systems, 13(9). https://doi.org/10.1029/2021MS002534

Hatfield, S., Chantry, M., Dueben, P., Lopez, P., Geer, A., & Palmer, T. (2021). Building Tangent-Linear and Adjoint Models for Data Assimilation With Neural Networks. In Journal of Advances in Modeling Earth Systems (Vol. 13, Issue 9). American Geophysical Union (AGU). https://doi.org/10.1029/2021ms002521

Kasim, M. F., Watson-Parris, D., Deaconu, L., Oliver, S., Hatfield, P., Froula, D. H., Gregori, G., Jarvis, M., Khatiwala, S., Korenaga, J., Topp-Mugglestone, J., Viezzer, E., & Vinko, S. M. (2020). Building high accuracy emulators for scientific simulations with deep neural architecture search. *ArXiv:2001.08055 [Physics, Stat]*. http://arxiv.org/abs/2001.08055

Kochkov, D., Smith, J. A., Alieva, A., Wang, Q., Brenner, M. P., & Hoyer, S. (2021). Machine learning–accelerated computational fluid dynamics. In Proceedings of the National Academy of Sciences (Vol. 118, Issue 21, p. e2101784118). Proceedings of the National Academy of Sciences. https://doi.org/10.1073/pnas.2101784118

Lary, D. J., Alavi, A. H., Gandomi, A. H., & Walker, A. L. (2016). Machine learning in geosciences and remote sensing. In Geoscience Frontiers (Vol. 7, Issue 1, pp. 3–10). Elsevier BV. https://doi.org/10.1016/j.gsf.2015.07.003

Magiera, J., Ray, D., Hesthaven, J. S., & Rohde, C. (2020). Constraint-aware neural networks for Riemann problems. In Journal of Computational Physics (Vol. 409, p. 109345). Elsevier BV. https://doi.org/10.1016/j.jcp.2020.109345

Nonnenmacher, M., & Greenberg, D. S. (2021). Deep Emulators for Differentiation, Forecasting, and Parametrization in Earth Science Simulators. In Journal of Advances in Modeling Earth Systems (Vol. 13, Issue 7). American Geophysical Union (AGU). https://doi.org/10.1029/2021ms002554

Ott, J., Pritchard, M., Best, N., Linstead, E., Curcic, M., & Baldi, P. (2020). A fortran-keras deep learning bridge for scientific computing. Scientific Programming, 2020, 1–13. https://doi.org/10.1155/2020/8888811

Partee et al. (2021). Using Machine Learning at Scale in HPC Simulations with SmartSim: An Application to Ocean Climate Modeling. arXiv:2104.09355.

Salter, J. M., & Williamson, D. (2016). A comparison of statistical emulation methodologies for multi-wave calibration of environmental models. *Environmetrics*, *27*(8), 507–523. https://doi.org/10.1002/env.2405

Schneider, T., Lan, S., Stuart, A., & Teixeira, J. (2017). Earth system modeling 2. 0: A blueprint for models that learn from observations and targeted high-resolution simulations. *Geophysical Research Letters*, *44*(24). https://doi.org/10.1002/2017GL076101

Stengel, K., Glaws, A., Hettinger, D., & King, R. N. (2020). Adversarial super-resolution of climatological wind and solar data. Proceedings of the National Academy of Sciences, 117(29), 16805–16815. https://doi.org/10.1073/pnas.1918964117

Williamson, D. B., Blaker, A. T., & Sinha, B. (2017). Tuning without over-tuning: Parametric uncertainty quantification for the NEMO ocean model. *Geoscientific Model Development*, *10*(4), 1789–1816. https://doi.org/10.5194/gmd-10-1789-2017

Zanna, L., & Bolton, T. (2020). Data-Driven Equation Discovery of Ocean Mesoscale Closures. In Geophysical Research Letters (Vol. 47, Issue 17). American Geophysical Union (AGU). https://doi.org/10.1029/2020gl088376

Zanna, L., & Bolton, T. (2021). Deep learning of unresolved turbulent ocean processes in climate models. In G. Camps-Valls, D. Tuia, X. X. Zhu, & M. Reichstein (Eds.), *Deep Learning for the Earth Sciences* (1st ed., pp. 298–306). Wiley. https://doi.org/10.1002/9781119646181.ch20

Zhuang, J., Kochkov, D., Bar-Sinai, Y., Brenner, M. P., & Hoyer, S. (2021). Learned discretizations for passive scalar advection in a two-dimensional turbulent flow. *Physical Review Fluids*, *6*(6), 064605. https://doi.org/10.1103/PhysRevFluids.6.064605

14 Tools

14.1 Introduction

Users require access to a number of tools and guidance material in order to make effective and efficient use of NEMO. With so many potential applications and use cases, it is important to determine what can be supported as part of a central development strategy. At the very least, the strategy must empower the community to support itself by providing frameworks for the discovery and retention of supporting software and documentation. This chapter describes the current provision and its most likely evolution.

14.2 Code repositories and web information systems

The most basic requirement is that users and developers have access to version-controlled code in a public facing repository. The enforced (but timely) move from the IPSL-hosted subversion server to a GitLab server hosted by Mercator Ocean provides a modern, long-lasting solution to the basic need and supports additional services.

This repository remains the central location for the traditional release branches and main trunk. However, the Git-enabled ability to fork the entire repository into an independent (but still traceable) copy means that even the most speculative or fringe developments can maintain a managed pathway back into the central repository without impacting the central repository until deemed worthy.

Sites that have, in the past, maintained mirrored copies with local developments that rapidly slip out of phase with central changes should find better options for maintaining local developments whilst retaining the ability to return those developments to the central copy (or to other forked copies? TBC).

Beyond the basics, the main repository also needs to support bug reporting and feature requests with clear allocation of responsibilities and traceable resolutions. The GitLab issues functionality provides all the necessary infrastructure and it is unlikely any external solutions will be required for these aspects. Issue boards may also be used to pair issue tracking and project management for organising the annual workplan.

GitLab's wiki capabilities will be used to host project-based information as a replacement for the previous Trac-based wiki pages. It may be necessary to configure this as a Group wiki in order for anyone with the developer role to edit content. This, however, is a feature of GitLab Premium and may not be available as an option.

External services will continue to be used for user forums (discourse) and conversational, topic-based, exchanges between developers (zulip).

14.3 Makenemo and SETTE

The makenemo script will continue to be maintained as part of the system and will retain its underlying use of the FCM build system. The subset of FCM components actually used will be held as part of the NEMO repository to protect against external developments of FCM that may affect its compatibility. Architecture files in the form of templates for common compilers and versions for the major supercomputing platforms available to consortium members will also continue to be maintained.

The introduction of Domain Specific Language pre-processing is expected during the development period. Tools such as PSyclone have already been tested with NEMO and are likely to provide the best method of supporting NEMO on heterogeneous HPC platforms by, for example, refactoring code for use on GPUs. A method of adding PSyclone as a pre-processing step within makenemo has been developed and will form part of the default provision. **[Action: incorporate PSyclone into the makenemo build system]**

SETTE remains an important component of the development process. A SETTE suite capable of performing necessary tests on supported reference configurations on at least one HPC platform available to each consortium member will be provided. Developments for NEMO will continue to be considered ineligible for inclusion if they fail any SETTE tests.

SETTE has evolved into a more versatile testing system that can be adapted for tasks outside the required testing regime. Some further, limited development of its capabilities may continue in coordination with the recommendations of the Verification and Validation Working Group. **[Action: further evolution of SETTE to make it easier to incorporate additional test configurations]**

GitLab's Continuous Integration capabilities open up the possibly of more rigorous and routine testing. Options for regular deployment of tests to consortium member's HPC platforms via GitLab Runners will be explored. With minimal adaptation, the SETTE suite could be used in such a scenario. **[Action: explore GitLab Runners for deployment of larger scale, regular testing]**

14.4 Critical tools

DOMAINcfg: This tool allows the creation of a domain configuration file (domain_cfg.nc) containing the ocean domain information required to define an ocean configuration from scratch. **[Action: Maintain compatibility with any changes in vertical coordinate capabilities]**

WEIGHTS: This directory contains software for generating and manipulating interpolation weights for use with the Interpolation On the Fly (IOF) option. **[No actions expected]**

REBUILD_NEMO: This is a tool to rebuild NEMO output files from multiple processors (mesh_mask, restart or XIOS output files) into one file. **[Action: A refresh may be needed; especially if tiling changes impose a change in restart file organisation]**

14.5 External tools

NEMO benefits from sites and packages maintained by individuals and organisations outside of the NST. Important examples include:

CDFTOOLS is a diagnostic package written in fortran 90 for the analysis of NEMO model output, initialized in the frame of the DRAKKAR project (https://www.drakkar-ocean.eu/). https://github.com/pmathiot/CDFTOOLS_4.0_ISF

SOSIE is an interpolation package for NetCDF files (full description available https://brodeau.github.io/sosie/). It is mainly used to pre-process file in order to start a NEMO simulation or to post-process output files.

[Action: Maintain links to such externals in all documentation and user-guides]

14.6 Containers

The almost total control of NEMO via its namelists provides opportunities for NEMO to be deployed in containerised environments. A totally containerised version is of little interest, other than for demonstration purposes, but a containerised NEMO with externally mounted experiment directories may appeal to non-traditional users. This has been proposed as a way of empowering local users in developing countries to configure and use limited area models without needing all the usual computing infrastructure. Some container systems, such as Singularity, even allow containerised executables to link to external libraries. This makes containers a serious option even within established communities since a single compiled case can be moved between platforms and still utilise libraries that are optimised for specific hardware.

If support for containerisation continues, future releases of NEMO may include containerised versions, precompiled for the most common processor architectures. Containers may also enable wider testing as part of a Continuous Integration system by offering simpler deployment to a range of diverse HPC platforms.

[Action: Explore options for providing containerised versions with each official release]

15 Verification and Validation

WGLs: Mike Bell and Claire Levy

15.1 Introduction

The NEMO V&V roadmap written in 2020 provides a comprehensive assessment of the status, opportunities and priorities for improvement of the tools and processes for verification and validation by NEMO developers and the NEMO System Team. It includes proposals for relatively short-term development within a fairly general framework. The 2022-2026 strategy for V&V should start from a re-examination of these proposals based on scoping studies undertaken since then.

Rather than re-opening a wider discussion we should focus on specific plans for making progress on the issues/opportunities identified there.

15.2 The main actions

The **main actions** that were identified in the Roadmap (though not in the same order as presented there) were:

- To scope out the options and costs for transferring the NEMO web platform from an svn/Trac system for code management and documentation to one based on git. It has been decided to transition to a self-hosted platform based using GitLab. This action is being progressed as a priority because the current system is installed on obsolete systems that must be replaced. The choices that are being made will have a significant impact on the tools available for development, maintenance and validation of the NEMO code. Moving to GitLab will not drastically change how new features are added in the NEMO reference (switch from a commit command to a push command). However, it will allow us to set up a number of new features related to V&V (to improve the reliability of the review process and exchanges between developers, and enable more automatic systematic testing which could evolve into some form of Continuous Integration). It will take the NST and developers some time to adapt to and become comfortable with these new tools – this should be recognised in the Strategy.
- To improve the NEMO regression testing tools: At the moment, each change to the NEMO reference or any development branch must pass a quite complete set of regression tests implemented by the SETTE shell script (SETTE, the regression testing framework within NEMO). This script runs functional tests on most of the Reference configurations and a subset of the NEMO Demonstration/Test cases. Some "short-term" useful improvements to SETTE have been identified. Whatever the GitLab related tool to be used in the future, these SETTE improvements will be easily transferred into them. For the NDS 2022-2026 strategy we should: (a) agree whether our regression testing will continue to be based on SETTE (hopefully the answer is yes that we can aim for evolution rather than revolution) (b) firm up a plan for evolution of SETTE and (c) agree how NST staff will be allocated to this work. These plans might appear in the Tools chapter rather than the V&V chapter.
- Other improvements to the SETTE testing should then be considered:
    - Use of containers to make SETTE easier to transfer between systems.
    - Use of cylc (or a similar tool) to allow SETTE to test a wider range of options or to be run more quickly (using a large number of parallel tasks)

- o Re-organisation to make it easier to incorporate demonstration cases within SETTE testing (both by developers and as part of the SETTE tool).

All these improvements will need to be considered within the context of the new GitLab platform which by default includes tools to launch sets of automatic testing. As an example, the green light of a reviewer for acceptance of a new development could be automatically conditional on the successful result of such a testing/trusting tool.

- To move toward Continuous Integration: some interesting and powerful tools are available within GitLab that could be used to improve the NEMO development workflow and processes.
- To seek an approach to enable the incremental introduction of unit testing of the NEMO subroutines/modules: A unit testing framework could be developed to support tests at a module level. Simple test coding conventions such as a 'test_' prefix for each test could enable a unit testing framework to be used within the SETTE system to parse the code, orchestrate the subroutine tests and extract and analyse the results (e.g. differences from the expected results). The unit testing framework would need to provide tools to generate inputs (using USR configuration codes and random or analytical fields). Code developers would need to define input data, parameters, expected results and pass/fail criteria. The feasibility of this approach could be studied by trialling it for one or two "representative" modules. One of the main issues to address is how to define and implement the input fields for the representative modules.
- Testing of code "in situ" has significant advantages and could be achieved by running the code using USR configurations. There are choices to be made on whether we need logicals to turn off other processes (as in MPAS), how we document the results (e.g. using more formal methods as in FESOM) and how we incorporate the tests in regression checks. We should experiment with alternative approaches so that we find one that works well (balancing the cost and the importance).

15.3 Other issues/opportunities

MOM6 have pioneered a number of useful additional tests of the code. For example: checking symmetry properties (solutions should not depend on swapping i and j); checking that there are no inconsistencies in the dimensions of quantities used by the code.

Could we take more advantage from the test/demonstration cases – perhaps in collaboration with the COMMODORE community?

Could we make better use of the "real-world" validation carried out by CMCC, the Met Office and MOi? This was viewed as outside the scope of the V&V roadmap but at the moment it seems to be a missed opportunity (Perhaps it happens "anyway" but could it happen more shortly after new releases; what would be the costs and benefits?) The MOi (Mercator Ocean International) METOF Expert Team could perhaps play a rôle in coordinating this.

15.4 Important constraints

NEMO development has, for now, a workflow including some relevant verification and validation tests. Still, the need to improve this V&V shared practices is recognized by all developers as a high priority, both for developers (to facilitate and accelerate collaborative developments, and reduce the time spent on bug fixing) and for the users (to make the future releases more reliable).

These methodology improvements will improve NEMO and its development. It will also - even with more automatic processes - increase the time needed to finalise a development and include it in the NEMO reference. The choices made need to take into account their impact on the rate of progress by and the resources that need to be allocated to the NST.

16 Data Assimilation interfaces

WGL: Dan Lea

An observation operator utility has been developed within NEMO over more than 10 years and maintained primarily by the Met Office. Unfortunately, Mercator and CMCC have not made use of this code (though ECMWF does) and the research community has made little use of it. [NOC recently developed a COaST assessment tool; which calculates model / observation differences; it does not use the observation operator code]. In order to avoid internal duplication of effort, the Met Office will probably transfer to an observation operator based on the JEDI system, so there may not be a group willing to maintain the observation operator tool in future.

The incremental analysis update (IAU) code needs to be tidied up and adapted for RK3. This should be completed before the end of 2022. Again, it is not clear which groups use this code, but the Met Office will maintain the primary IAU option.

Is there a requirement for a tangent linear (or linearised perturbation) version of NEMO? The TAM code has not been updated since Version 3.6. but the NEMOVAR consortium have plans to develop 4DVAR capabilities using a more recent version of NEMO (probably 4.0.X) which will involve updating the TAM to be relevant to this later version.

The Mercator Ocean International Marine Data Assimilation (MDA) Expert Team has set up a working group to assess the feasibility of developing a shared MDA framework. The JEDI and PDAF frameworks will be considered as part of this study. The interface between NEMO and PDAF puts few constraints on the NEMO model, though to use NEMO within PDAF one would need to change the top-level NEMO subroutines. Were JEDI to be used as the framework, and the NEMO model itself run within JEDI, a JEDI-compatible interface between NEMO and the assimilation software would need to be developed and maintained. One would need to be able to restart the NEMO model from and output it as data in the form of the assimilation software's representation of the NEMO state vector.

17 NEMO Community support

WGLs: Authors: Stefania Ciliberti (CMCC), Jeffrey Polton (NOC), Mike Bell (UK MetOffice)

17.1 Introduction

Supporting users and enlarging the group of people using the NEMO ocean model for research and development as well as for operational framework is a key for the next generation of services and applications for the Blue Ocean. Being a community model, NEMO has already put in place some initiatives, devoted to providing comprehensive information about the mathematical model and numerical schemes as well as instructions to install and run a NEMO configuration.

The scope of this chapter is to develop a roadmap of potential actions for the NEMO Community Support to further improve dissemination capacity.

We focus on three main macro-categories:

- Documentation (including reference manuals and users guides)
- User forums
- Training activities

17.2 Documentation of model formulation

17.2.1 Current status

As of today, NEMO documentation is maintained by the Consortium members through the System Team and offered to users through the NEMO webpage https://www.nemo-ocean.eu/.

The NEMO website presents in particular 3 main sections for introducing NEMO and its modelling components:

1. Components: description of the NEMO modelling components (Core Engines); description of reference configurations and test cases with list of available setup and to Github repository (Reference Configurations and Test Cases); description of external tools like AGRIF, OBS, XIOS, SIREN with relevant links (Interfaces and Tools). This section provides, in particular, a general overview of the main components as implemented in the NEMO code.

2. User Guide: redirecting to NEMO User Area, a forge ipsl NEMO page, with links to documentation for available release(s) and other useful links for users (newsletter, Discourse for online forum). The NEMO User Area should provide a general overview on how to install, configure and run a complete NEMO configuration;

3. Reference Manuals description of user manuals and how to cite them. They include NEMO ocean engine, sea ice, and biogeochemistry components. It also reports previous versions of the documents. Documentation has specific DOIs and it is accessible through Zenodo service. It is available as pdf and as html.

The **Reference Manual** provides a comprehensive and scientifically-based description of the NEMO ocean model. It opens with disclaimer, list of other resources (website, development platform, repository for demonstration cases, online archive and newsletters links), how to cite rules and it comes with a DOI.

The manual outline lists the chapters of the reference manual: each chapter corresponds to a specific submodule of NEMO code (i.e., DOM for the space domain, TRA for ocean tracers, DYN for ocean dynamics, etc.) and reports a description of the numerical schemes as implemented in the code. Each chapter comes with a change record that tracks release, author(s) and modifications.

17.2.2 Strengths and Weakness analysis

Strengths

- Contents and documents as available on https://www.nemo-ocean.eu/doc/ are managed by the System Team. Each PI creates a ticket on the specific development: once completed, then the PI drafts the section/chapter which is then reviewed by the internal Reviewer before its publication. With this process, the contents of the reference manual are always kept updated and inline with the code release;

- Reference manual is available as html and pdf;

- Sections are clear and report mathematical model description, numerical schemes and corresponding routines as implemented in the NEMO code.

Weakness

- Due to high activity in the numerical modelling developments, the guides are not often entirely refreshed and they may not document completely all the major upgrades of the code. For example, at today “Surface Boundary Condition (SBC)” chapter as available in the online version still contains old information about bulk formulation (CORE, CLIO, MFS);

- Core engines, accessible through Home > Modelling Framework > Components > Core engines, are still linking to old NEMO versions. Accessing through the “Reference Manuals” the user is redirected to the new documentation as produced for the last NEMO release;

- Only a few of the chapters of the reference manual have clearly defined Chapter Leaders .

17.2.3 Proposals

Considering main users requirements and on the basis of the available platforms, documentation and contents developed by the NEMO community, we propose:

1. simplification of the access to scientific information through the NEMO website (short term objective)
2. maintenance and quality assurance of the scientific documentation (medium term objective) including identification of Chapters Leaders to work in connection with NEMO Project Managers and PIs

Regarding point 1, this could be easily achieved by rearranging the already existing material as available online and dedicating a section in the website that points to the reference manual.

- “Core Engines” should contain the description of the main NEMO components without extra links to manuals (today, we have duplication of the information since each engine links to the same reference manual). An updated version of the core engines picture could be also needed since the information here reported are not fully updated.

- “Reference Manuals” should contain the direct link to NEMO Reference Manual and other modelling components reference manuals, in pdf and html (if available). It could combine the already provided information as in the “How to cite” section. Additionally, it could provide an overall view of the NEMO code architecture as fully described in the manual.
- “User Guide” is misplaced, since the technical information are part of the “Download & Install” section.

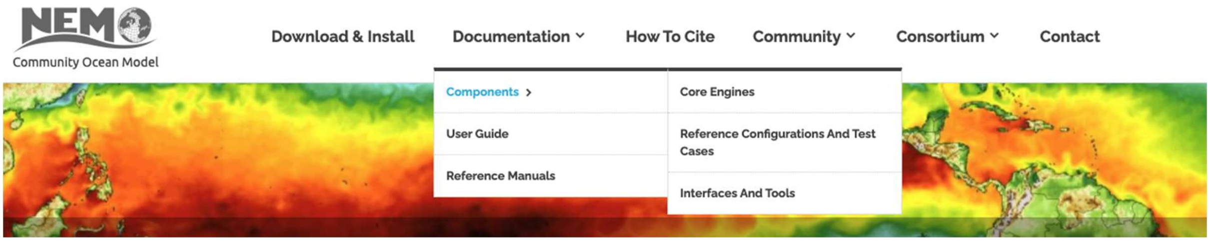


Figure 1 - Main menu of the NEMO website

Regarding point 2, the main actions should be devoted to setting up a method for editing, quality control of the scientific contents and evolutions of the reference manuals. The website should offer to users the last updated version of documentation and code at a glance. Old versions, valuable from the scientific point of view, can be hosted in a dedicated section of the website, avoiding overlapping with new information that may confuse the users. This action can be organised through the implementation of a documentation management system. A collaborative framework may help in organizing and tracking the document lifecycle, facilitating its update and supporting the PI in revising it for the final delivery/publication.

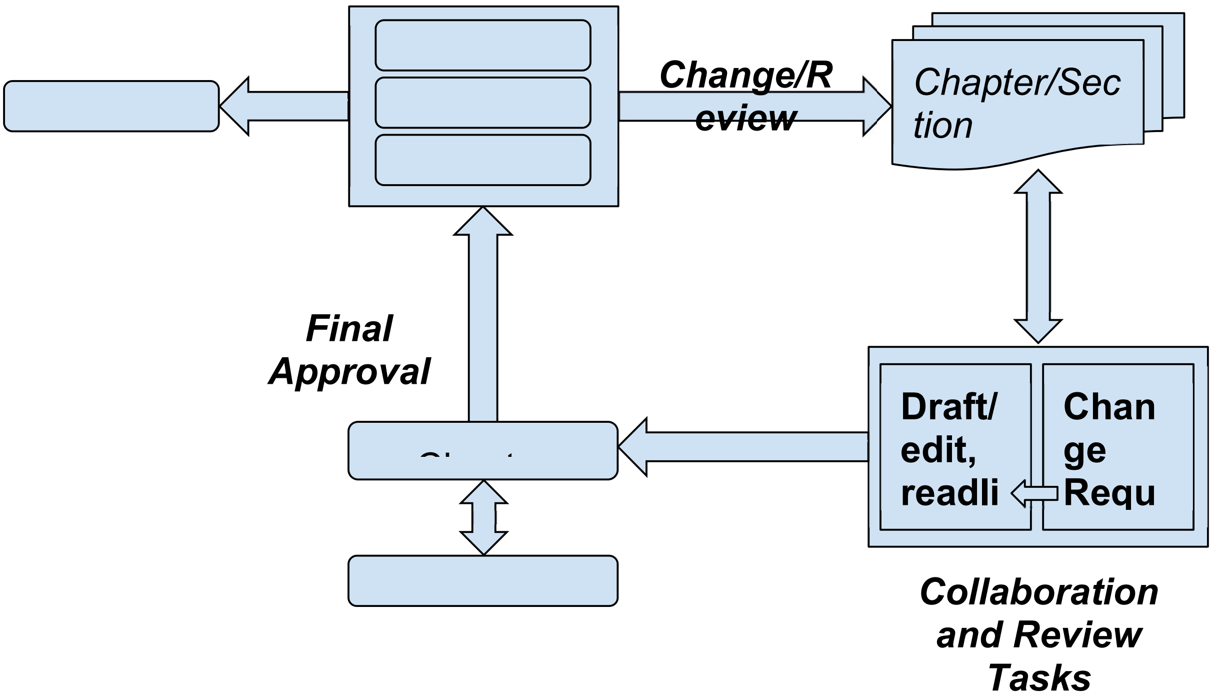


Figure 2 - Collaborative workflow for scientific contents preparation

As shown in Figure 2, NEMO Project Manager, Working Groups Leaders and Developers could ask for a change/review process for a specific chapter/section. A template could be made available on an online platform (Google Drive?, Alfresco?, or other kind of solutions that can be discussed by Consortium Members) in order to promote collaboration among Authors and co-Authors. The drafting phase can start once the change request has been approved by the Chapter Leader: it includes draft preparation, edit, readline, review and approval. The process ends once the Chapter Leader, in agreement with co-Authors, finally approves the change and sends it back to the NEMO Project Manager for the final push to users.

A Documentation Manager could be nominated to support the NEMO Project Manager and Chapter Leaders for the organization of the tasks: a dedicated action in the Yearly Workplan could be set up in order to plan what kind of changes the reference manual will need.

17.3 User guides & demonstrations

17.3.1 Current status

NEMO provides a Users Area https://forge.ipsl.jussieu.fr/nemo/wiki/Users, whose aim is to provide a complete description of the state-of-the-art NEMO modelling framework and of related engines. It offers the following functionalities:

- link to documentation of official releases (https://forge.ipsl.jussieu.fr/nemo/chrome/site/doc/NEMO/guide/html/install.html)
- technical support for help on:
    - login issues
    - creation of ticket
    - bookmarking favourite resources
    - customizing email notifications
    - access to Discourse https://nemo-ocean.discourse.group/
- newsletter and informative section on NEMO development activities

The Users guides as available for example here

https://forge.ipsl.jussieu.fr/nemo/chrome/site/doc/NEMO/guide/html/install.html

provide in particular information about system requirements, how to extract and install XIOS and NEMO, how to create and compile a new configuration, run it and use CPP keys.

17.3.2 Strengths and Weaknesses

Strengths

- The overall organization structure of the online section offers quite robust information on the supporting capabilities of the NEMO Community. Online tools - e.g., Discourse, tickets - help users to address potential problems and solutions directly to developers and benefit from their feedback.
- Available documentation is a good starting point for users. Information as accessed through "Documentation & Install" can be used by users to download, compile and run a NEMO configuration. It also provides a description of the available reference configurations and list of working ones, with links to input data to use for their executions.

Weakness

- Missing section summarising the main changes between versions or releases.
- Missing section on the results expected from reference configurations

17.3.3 Proposals

Designing the next user corner with running examples/demonstrators able to provide:

- Scientific description of reference configurations, including results to be used by users to validate results
- External tools capacities and functionality, with demonstration on their usability

17.4 User forums

As of today, the NEMO Community offers the Discourse platform for exchanging information among users and developers. This new platform is a major improvement on the previous Forum and is being very actively used. It is being used to

- address issues as faced in the working releases
- support users for the usage of the code, configurations and demonstrators
- answer user questions
- understand the users needs for potential new developments

17.4.1 10.4.1. Proposals

The NEMO System Team should continue to support and evolve its use of the Discourse platform.

17.5 Training (for users and developers; on-the-job & courses; continuous development)

Supporting the scientific and research community is key for the development of the NEMO code and community. Academia may greatly benefit from the advancements of NEMO from the numerical point of view. Similarly the NEMO code base could greatly benefit from Academia engaging more closely with, or leading aspects of its development. For this reason, the next phase should enforce links between NEMO community and R&D groups, operational centers and Academia.

There are several tiers of NEMO proficiency that are exhibited in users of the NEMO system. Not all new users require advanced developer's skills. Similarly, not all new users will require introductory training. In the following, "training" is interpreted in a very broad sense to be provision of material that accelerates an individual's ability to make progress with NEMO in such a way that they could help others to the same.

Typically a user would be anticipated to grow in skill level with time and therefore training would be expected to match the requirements and skills level of the participants.

17.5.1 Overview of established approach and provision

The current approach to training provision comes from four main directions: firstly, centralised NEMO provision through documentation (16.2) and centrally hosted user guides (16.3), which are discussed above. However at present they are very technical in nature. Secondly, locally managed provision; thirdly community driven support, and finally workshops. In this discussion locally managed training is delivered peer-to-peer whereas community driven support represents a one-way exchange of user defined information through web based technologies.

17.5.1.1.1 NEMO documentation

Online tutorials can be a valuable tool for training purposes especially for beginners. The current documentation is, by contrast, pitched as a technical reference manual. This is essential, however there is also room for basic tutorials on:

1. How to compile and run NEMO for setting up a realistic configuration
2. Introductions to core engines, with discussion on the rationale for how and why,
3. Information highlighting the main novelties and updates offered by NEMO.

17.5.1.1.2 Locally managed (peer-to-peer) provision

For pragmatic reasons it is observed that research groups tend to persist with the modelling tools they know. Hence NEMO groups use NEMO, and e.g. MITgcm groups use MITgcm. In this way, it is largely down to individual modelling teams to determine how they:

- Upskill new modellers in their groups;
- Resolve issues around skills gaps within their group;
- Support continuous development and learning.

Typically in this model, training is gleaned from key individuals who serve as “fountains of knowledge” or mentors. In some instances these individuals might typically also be on the NEMO System Team. The experienced individual will work with colleagues giving them working examples (configured for their architecture), and introductory guidance on how to get started (this is the namelist, change these timestepping parameters / forcing files / etc). The “apprentice” will gradually learn as they go and receive tailored guidance according to their knowledge and skill requirements.

Caution: This on-the-job apprenticeship approach is more sustainable in large modelling teams, where natural turn-over of staff can be locally enriching (bringing new HPC techniques or analysis techniques and export NEMO expertise elsewhere) rather than devastating (e.g. in the loss of a single key individual) to the group’s skill base. For small research groups in Academia, where there is no top down strategic support for NEMO, this situation presents a high risk barrier to engagement with NEMO.

17.5.1.1.3 Community driven support (web based content)

There are potentially significant overlaps between Locally Managed Support and Community Driven Support, when for example Locally Managed Support is put on-line. The distinction here is made that Community Driven Support encompasses the user-defined web-based documentation. This ad hoc content typically addresses the following types of problems, in the form of user written notes:

- How to compile and run NEMO on particular architectures,
- How to set up realistic regional configurations
- Community built tools that facilitate pre and post-processing data

Examples of this include:

- A long history of tools for building and configuring regional models:
    - https://pynemo.readthedocs.io/en/latest/examples.html#example-2-lighthouse-reef (2015)

    - https://github.com/PyNEMO (2021)
- Guidance for building NEMO regional models: https://github.com/NOC-MSM/NEMO-RELOC/wiki

Alternatively well-resourced long-term projects that truly embrace the open source philosophy have invested heavily in well documented materials:

- *the Salish Sea Marine Environmental Observation Prediction and Response MEOP* project and documentation:

  https://salishsea-meopar-docs.readthedocs.io/en/latest/code-notes/salishsea-nemo/quickstart/index.html

- *The Structured and Unstructured grid Relocatable ocean platform for Forecasting (SURF),* developed by University of Bologna in collaboration with CMCC:

  https://www.surf-platform.org/

Google reveals other individuals, who publish their NEMO "how-to" notes online. These are a valuable resource for individuals who follow similar paths (typically architecture settings), as well as being valuable to the author.

17.5.2 Workshops

When a number of individuals require simultaneous upskilling institutions and organisations have been known to deliver NEMO specific training through workshop formats. The true extent to which workshops are run institutionally is hard to ascertain. However the following are workshops known to the authors:

- An introduction to ocean modelling: Running NEMO in Docker
    - target: interested environmental scientists with command line access to their laptop. Run twice (Belize, Merida)
- Coastal Ocean Assessment Toolkit: Python diagnostics package for high resolution regional NEMO model
    - target: new NEMO data users / potential NEMO diagnostics developers. Run several times in the UK. Hosted by the UK Joint Marine Modelling Programme.
- Relocatable NEMO: how to build and configure regional NEMO model
    - target: scientists who want to do this, but have been put off, or haven't yet. This was organised, to be hosted by UK Joint Marine Modelling Programme. It had significant UK interest but was postponed indefinitely.
- Expert Team for Operational Ocean Forecasting (ETOOFS), joint IOC-WMO and GOOS: the Southeastern Brazilian coastal model (https://www.surf-platform.org/tutorial.php)
    - target: students and scientists who want to learn on how to setup an operational ocean forecasting system by using NEMO (organized by ETOOFS https://www.goosocean.org/index.php?option=com_oe&task=viewGroupRecord&groupID=198 with University of Bologna and CMCC).

Historically these were designed and delivered within organisations, though the COVID19 pandemic broadened the potential reach of this type of content, which is well received.

The workshops are constructed around web based material.

Strengths

- Providing a point in time where users can schedule the often delayed learning of new skills.
- Material exists beyond the workshop, providing as a point of reference for the delegates for subsequent implementation.
- Builds community
- People can attend with a range of intentions. Some are managers that want to know if they should delegate, some come to listen to make an assessment if they want to commit, some come and actively follow along because they need to learn ASAP.
- Material is very recyclable and updateable.

17.5.3 Practical steps to improve current provision

Much of the training material described above is not managed centrally, or formally, by the NEMO Consortium. This is a strength in that the training is managed dynamically and targeted according to demand but it is also a weakness for NEMO users who do not have access to these dynamic networks, which largely sit within consortium members.

As a first practical step, the Consortium could **catalogue a collection of active online resources**. These could be sorted into genres:

- how-to guides;
- useful external tools;
- NEMO projects
- etc

The catalogue would require time-stamps on the links, so that obvious problems associated with aging links would be apparent to the reader. Users would be encouraged to volunteer hyperlinked content, perhaps annually, at which point old links could also be "moved down the list" or archived.

As a second practical step, online **workshops** could be advertised and offered more widely across the user community. Some consideration would need to be given on whether the offered material should be endorsed by the Consortium, perhaps successful workshops could be invited by System Team members? Some initial trialling of the above would determine the size of appetite amongst the user community for delivering and receiving workshop material, and whether, or how, it needs to be costed.

The third practical step would be to freshen up the **web offering** with a regard that the reader may not yet have decided to use NEMO, or maybe very new to NEMO. Attention should be focused on the "Getting Started" topic; making these materials easier to find and adopting the "worked example lecture approach". In addition, **quarterly updates** should be used to advertise the latest developments, perhaps in the form of informative/multimedial material. These could be simultaneously targeted at both the NEMO and broader community, in order to advertise NEMO progress and developments.

17.5.4 A road-map: medium term goals and short term direction of travel to head there.

Following a suitable trial period, the value of endorsed external training materials should be reviewed. If it is found to be central for the uptake by new users or the continuous development of existing users then more permanent adoption (and support) of methods and materials should be provisioned.

If the Consortium identifies that supporting the scientific and research community is a key for the development of the NEMO code and community, the next phase should purposefully seek to enhance links between NEMO community and R&D groups, and between operational centers and Academia. In order to later benefit from the engagement with global Academia, the Consortium could set its sights broad and aim to be the “Nearly Everywhere Model for the Ocean”.

17.6 Summary and recommendations

- Need to dedicate System Team / Core resources to actively monitoring the pulse of the Discourse and to then reactively updating static documentation (manuals/user-guides). Initially delivery on this would be for a sustainable work flow plan.
- Review this document in light of feedback sought from wider community users (up to Jun 2022).
- Establish a method for documentation revision in order to be aligned with code versions.
- The Consortium should ‘endorse’ selected external training material as a pragmatic way to minimise overhead of managing new training offerings whilst rewarding contributors of material.
- Review the Getting Started material to include worked example tutorials.
- Advertise NEMO progress and developments quarterly.
- The Discourse platform for exchanging information among users and developers is an excellent new development and a great step forward in our abilities to engage across the community of users. It is, however, too early to critically review.