Elements of the NEMO prospective : CNRS-INSU contribution

This document is not CNRS-INSU's precise workplan but a list suggestions of what should be tackled considering the known model deficiencies and needs expressed by the NEMO-CNRS-INSU community.

CNRS-INSU (Institut National des Sciences de l'Univers), in its "ocean atmosphere" sector, gathers joint laboratories from CNRS, universities and other institutes covering all aspects of ocean physics, ocean biogeochemistry and sea ice. INSU is the main institute responsible for the maintenance of NEMO as a "shared modelling platform". NEMO is currently used for research in a number of INSU laboratories and beyond in the French research community, for example:

- NEMO is the ocean-ice-biogeochemistry component of the two French Earth System Models contributing to IPCC. For CMIP5, IPSL contributed long experiments using the ORCA2 global model and CNRM-CERFACS contributed to the decadal scenarios using ORCA1.
- At the global scale, eddy-permitting and eddy resolving NEMO simulations are produced by the DRAKKAR project and shared with the community (www.drakkar-ocean.eu).
- High resolution regional configurations are developed, often by using the AGRIF grid refinement (recently: the Salomon sea, the Arabian sea, the Mediterranean sea...)
- Ocean-atmosphere coupling at high resolution is developed to investigate processes and building climate scenarios at the regional scale.
- Coupled ocean/biogeochemistry simulations are performed and analyzed as part of Earth System Modelling efforts (IPCC) or, at high resolution, within the TANGGO consortium in collaboration with MERCATOR-Ocean.
- NEMO is used in idealized model configurations (e.g., the rectangular basin GYRE configuration), to investigate specific processes.

In the CNRS-INSU community, the targeted applications at a 10 years horizon are quite numerous and ambitious. They can be summarized as follows:

A coupled ocean, marine biogeochemistry and sea-ice (Blue-White-Green, BWG) framework having a *forced* and a *coupled* interface with atmosphere (and its chemistry), surface waves, ice sheet / icebergs and land. The framework, flexible enough to be used with one or a few compartments, should be applied

- at global scale with horizontal resolution 2°-1° (Paleo), 1/4° (CMIP6), 1/12° to 1/36°, and O(100) levels (at least 1 meter at the surface).
- at regional / coastal scale with horizontal resolution ranging from 1/12° to a kilometre and O(100) levels.

Such BWG framework should include AGRIF grid refinement capabilities, will be used as a whole or in sub-set, and would be used in a data assimilation context (variational or stochastic) for forecasting, parameter estimation, sensitivity analysis, design of new parameterizations.

To reach these goals, progresses have to be made in numeric and physics of all NEMO compartment (in particular with the increase in resolution) as well as in exiting and new interfaces (AGRIF, atmosphere, biogeochemistry, land, wave model, ice sheet…), and a new compartment have to be created (sea-ice biogeochemistry).

CNRS-INSU laboratories are using NEMO for grand challenges on super-computing centres (Earth Simulator in Japan, GENCI in France, or the European infrastructure PRACE). It is necessary that NEMO remains competitive on supercomputers in the future, thus the High Performance Computing strategy is also a priority.

A full list of suggestions collected in the INSU community is given in the Appendix. From these suggestions our main priorities are the following:

0. System environment :

(1) versatile tool to set up and run targeted configurations (global, or regional configurations with AGRIF grid refinements) in an ESM framework

(2) integrated system (multi-components) but preserve stand alone capabilities for each part: preserve the physical & numerical upgradability of each individual component

(3) provide a new suite of validated test cases (legacy of the french ANR project COMODO, *www.comodo-ocean.fr*)

(4) promote the use of data assimilation techniques via demonstrators and tutorials for assimilation, parameter estimation, development of a parameterization, or model analyses. NB: the development of assimilation techniques by themselves is out of the scope of NEMO.

(5) maintain the Tangent & Adjoint Models (TAM) in phase with the dynamics, and possibly extend it to some other components.

1. Ocean kernel:

(1) evolution of ocean numerics in both time and space (better adaptation to targeted high resolution, with better control of implicit numerical diffusion)

(2) use of mixed vertical coordinate: z-s-ALE (i.e. terrain following/partial cells/Arbitrary Lagrangian Eulerian) in global configurations to better represent the overflows, the bottom boundary layer, and explicitly represent tides.

(3) cut-cells technique and development of time-varying cut-cells to better represent de complex geometry of ocean basins and the time-variation of under-iceshelf cavities.

2. ocean physics

(1) waves in the system. This require changes in ocean dynamics, physics, and surface fluxes (bulk formulae, gas exchange), and an interface to an external wave model.

(2) downscaling of the atmospheric forcing at ocean scale via a coupling to an atmospheric boundary layer model: better force an eddying ocean.

(3) better representation of the cold ocean sphere : from dense water *formation* (polynia, air-sea-ice sheet interactions), interior *transformation* (overflows, bottom boundary layer), and *consumption* (internal tides, lee waves, and near inertial wind driven internal waves and their associated interior mixing)

3. Sea-ice (LIM-3)

(1) creation of a BGC compartment for LIM sea-ice and its interface to PISCES (potentially interfaced to others sea-ice and BGC models)

(2) rheology and thermodynamics adapted to higher resolution, physics of air-ice-sea interaction, snow compartment.

4. BioGeoChemistry (BGC)

(1) Super-parameterization of the ocean for BGC (higher horizontal resolution on ocean than on BGC): allow the use of BGC in very large configurations at reasonable coast without significant alteration of the results

(2) re-design ocean-BGC interface: sinking of particles in the ocean transport part. Only the source-minus-sink terms will remain in the BGC model

(3) management of carbon and nutrient fluxes provided by land models

5. Grid refinement (AGRIF)

Improved of AGRIF maintenance, robustness, and versatility

(1) enable different vertical grids & coordinate systems between mother and child grid(s)

(2) improve AGRIF robustness (AGRIF library base on open source lexical analyzer)

6. High performance Computing

NEMO is currently achieving reasonable performances on 10k cores. Some "tricks" could be added to reach a maximum of 100k cores. However it is clear that the parallelisation of the code is not good enough to go beyond this limit and take advantage of the new architecture of the machines (> million of cores) expected in the coming 5 to 10 years. A deep reorganization of the code has to be expected. Knowing it will represent a big amount of work and impact the whole NEMO community, this action should start with a rigorous and complete audit of the solutions existing or considered by other modeling groups (WRF, GFDL, CESM, ROMS...) and HPC experts (computing center and manufacturers). A working group gathering physicists and HPC experts is needed. An action is starting in France with Bull/Intel in the frame of their "center for excellence in parallel computing" and with Nvidia using OpenACC. Links with "la maison de la simulation" may be possible.

7. Code maintenance and user support

The question of the code maintenance and the user support should not be omitted as it is needed and can potentially represent a large amount of work. The code maintenance (compatibility and tests of the different options, code consistency and readability) is a key point to maintain the quality of the code which is (was?) part of its success. User support can represent a large variety of task: emails, forums, user meetings, on line or on site tutorials, specific documentations and publications… A clear decision of what we want to do and what we can/cannot afford is needed to know which equilibrium between developments and maintenance we are targeting.

APPENDIX

This appendix provides a list of suggestions, classified by system components, that has been collected among the INSU community.

I. Ocean component

I.1 Global ocean component (climate, DRAKKAR):

• Increase of resolution (from 1/4° to 1/12°and 1/36°)

- higher order temporal/spatial schemes (increase of effective resolution) to better account for non-linearities that appears in the system with increasing resolution
  - 3rd order scheme with the diffusive part acting along isoneutral surfaces (Lemarié et al. 2012).
  - development of a 3rd order scheme for vector invariant momentum advection.
  - explore other schemes, in particular for the vertical (5th order, compact or exponential compact schemes (Tian and Daï 2007), …)
  - time stepping: from LF-RA to a higher order scheme which satisfies the constraints set by other compartments (BGC, AGRIF, on-line coarsening). Joint space-time approach to benefit of self compensation of dispersive error in time and space
- Keep reasonable size for the I/O : on-line coarsening of the outputs including 2nd order moments (to be done at the I/O server level?)

• Improved physics :

- air-sea interactions: downscaling of the atmospheric forcing at the ocean scale (on-line coupling with an atmospheric boundary layer running on the same horizontal grid as the ocean.
- surface wave in the system: impact on surface dynamics, mixing, and air-sea fluxes
- overflows: use of mixed partial cell / terrain following vertical coordinate system ; explicit representation of the bottom boundary layers ; explicit representation in key areas (AGRIF zooms)
- tides in the system and their induced vertical mixing: explicit versus parameterization?
  explicit: use of z-/s-tilde coordinate (minimization of numerical mixing). However, how to parameterize the short unresolved internal waves? How to deal with the tide-aliased outputs?
  parameterization: currently only the short internal waves that dissipated in vicinity of the generation site are parameterized. How to represent of the long waves mixing?
- ocean boundary layer : turbulent closure versus new formulation ; restratification effect of sub-mesoscale ; etc.
- development of a new open-sea ocean deep convection parameterization and re-activation of the non-penetrative convective adjustment algorithm
- Physics of intermediate resolution O(1/4°) : eddy induced restratification when local radius of deformation becomes lower than Δx, parameterization of eddy steering, stochastic parameterization…

- Develop new parameterizations for the dynamics near the lateral boundaries in the case of partial steps (perhaps in association with new numeric, immersed boundaries, etc?)

• coupled air-sea interface: downscaling of the atmospheric forcing at the ocean scale in coupled mode.

• possible development of a lake model based on NEMO including ocean, biogeochemistry, ice and sediment: useful for global and regional configurations

I.2 Global Ocean component (paleoclimate):

Paleoclimate specificities : coarse resolution (1° or 2° spatial resolution) + parameterizations of many processes (eddy and sub-mesoscale restratification, convection, overflows, tidal mixing, ice sheet - ocean interactions…) + use of different positions of continents + very long simulations (glacial interglacial period O(10,000 years) and more) + represent the 0(100 m) changes in sea level and its associated changes in coastline + coupling with ice sheet (including iceberg calving).

• adapt ocean physics evolution for low resolution, in particular:
  - overflows, tidal & wind induced mixing, iceshelf, submesoscale, space and time varying eddy induced coefficient...
• explicit representation of the cycle of tracers used as proxies (isotopes of O_2, Carbon, …)
• management large change in sea-level (i.e. ~150 m):
  - time evolving coastline (adapt the technique developed for time-varying ocean cavities)
  - non-linear sea-surface (i.e. ocean level scale with sea level)
• position of mesh poles: continental drift issue
  - management of cubic sphere mesh (its 8 singulars grid points : finite volume approach)
• HPC : improved computational efficiency for small size but long simulations
  - coarse grain parallelism with OpenMP (momentum and tracer threads, for example), masking of communication with computation, use of GPU (OpenACC)…

I.3 Regional/Coastal Ocean component:

• setting : fast and accurate setting of regional and coastal configurations (CFG manager) including sea-ice, BGC and coupled interface to atmosphere, waves, and land. Consider the possibility of generation of curvilinear (orthogonal) grids adapted to the coastal boundary (enabling grid refinement in estuarine areas, straits, etc.... limitation of the number of grid points in the land mask)

• open boundary condition (OBC) : management of ocean, tides, sea-ice, and BGC at the boundary. (N.B. need of ocean reanalyses that include a BGC component) ; need OBC (and AGRIF grid refinement) that account for z-/s-tilde (ALE) vertical coordinate.

• downscaling of the forcing at coastal scale (see global eddy resolving issues)

• better fit of the coastline: cut-cell approach or immersed boundary (this is also important for global models) combined to a better use of the curvilinear grid capabilities (when possible).

• wetting and drying associated with tides. Classical approach versus time evolving coastlines? Specifications: preserve the conservation properties, avoid too intrusive approach, ensure compatibility with OBC

• s-coordinate or mixte z-/s-coordinate: for reduction of the number of vertical levels in very shallow areas (CFL considerations), reduction of the pressure gradient errors over steep bathymetry.

- rotation of the diffusive part of high order advective operator along neutral surfaces (Lemarié et al. 2012a,b)
- pressure gradient computation in non-geopotential coordinate: keep in phase with the coastal modeling community (in particular the COMODO group)

• non-hydrostatic: progress on outstanding issues (before starting implementation in NEMO): (1) classical approach (Poisson solver) versus new approaches (pressure propagation in Non Boussinesq models) ?; (2): all components of the Coriolis acceleration ? (3): Time splitting: methods to reduce the numerical cost of the (NH) free-surface ?

• sediment model : As part of NEMO or interfaced with an external sediment compartment? Offline calculus?

I.4 Ocean kernel

Rq : default setting: from low order schemes, linear free surface, zps-coordinate system to high order time-space scheme, non-linear free-surface, zps-s-tilde mixed coordinate.

• possible evolution toward unstructured ocean kernel ?

Replacing AGRIF zoom by local change in resolution is an attractive feature, but: need ocean physics that adjust itself to change in resolution, difficulties in using different algorithms/operator depending on resolution as its is possible with AGRIF. Moreover, an on-line coarsening of BGC becomes problematic, not to say impossible…

==>> better to think of two-way coupled interface between coastal/littoral unstructured models and NEMO rather than moving to an unstructured kernel.

==>> wait for a more mature solution before thinking to move toward unstructured model. Nevertheless, move interfaces when possible to obtain pieces of NEMO system that are independent from the type of kernel (Source minus Sink terms of BGC model, thermodynamics of sea-ice, iceberg floats, vertical mixing (TKE, IF-less KPP, GLS), iceberg floats,…) and promote their use in unstructured framework.

• equation of state : TEOS10 for boussinesq (and non-Boussinesq?) fluids

• Improved and reliable diagnostics ("sanity checks") for conservation of tracers, energy, etc

• relax the non-Boussinesq approximation (?) (U --> 〉/〉o U and associated changes in continuity equation, pressure instead of depth coordinate): mass conservation instead of volume conservation for a explicit representation of steric mean sea level

• HPC :

- reduction of memory access (e.g. divergence of a flux computed in single loop, predefined surface cells, thickness weighted tendencies, …)
- more efficient split-explicit time stepping for the external mode computation (larger of barotropic time step, larger overlap area for less communication, …)
- use of larger Δt and domain for low latitude processors than for high latitude processors
- distributed on-line diagnostics: I/O server

II. AGRIF : two-way local grid refinement

II.1 Main axes of development

• Allow different vertical grids & coordinates system between mother and child grid(s)

• Developments: towards an overlapping composite grids system

- capability to run several AGRIF zoom at the same time in parallel
- ocean time stepping:
  (a) better fit AGRIF requirements (get rid of Asselin time filter)
  (b) AGRIF compatibility with split-explicit (non-linear) free-surface (1st step: mother-child update at mother master time step ; 2nd step: mother-child updates at mother external time splitting time step (see ROMS)
  (c) AGRIF compatibility with Elasto-Visco-Plastic (EVP) rheology (same issue as split-explicit free-surface)
- introduction of direct interactions between overlapping child grid having a same factor of refinement.

• Development of the AGRIF library (same idea regarding TAM):

- invest in a new pre-processor based on existing open source lexical analyzer (having already a knowledge of FORTRAN) rather than the current homemade one.
- adapt as much as possible the ocean code to minimize the work done by AGRIF preprocessor ==>> minimize the number of issues encountered when checking the compatibility of a new release with AGRIF

• Assimilation and local grid refinements :

- assessment of data assimilation (with sequential or variational methods) when an AGRIF zoom is present in the model configuration.

II.2 Minor points

- AGRIF robustness : improve AGRIF stability through an evolution of the algorithm used in mother-child overlap areas.
- AGRIF able to cross east-west cyclic boundary and north fold conditions
- filtered free-surface and AGRIF: use of a multi-grid solver to solve all together the elliptic problem?
- update of mother grid: ensure that the model output on the mother grid over the child area are consistent with what is actually computed in the child.
- freshwater budget correction: the correction should come from the *mother* grid
- Nesting tools : introduce properly a space variation of the scale factor in the child grid
- assessment of ALE vertical coordinate with AGRIF
- iceberg floats and AGRIF

II. Biogeochemical component :

• PISCES evolution

- evolution of PISCES kernel as a quota model
- diurnal cycle: move from daily PAR to explicit resolution of the diurnal cycle in PISCES (will need the quota model)
- end-to-end : add APECOSM to represent upper trophic-levels (and replace the

zooplankton closure scheme)

- sediment / benthos compartment for coastal/littoral application ?
- modular PISCES: Today, only 2 BGC modules of different complexity are included in PISCES: full PISCES (24 tracers) and LOBSTER (7 tracers). This could be made much more modular by derivating a few configurations of the PISCES module depending both on the biogeochemical characteristics of the region considered, and on the scientific question raised.

Examples of modular version of PISCES could include (not exhaustive): PISCES-NPZD-nocarbon : 7 tracers ; PISCES-NPZD-w/carbon : 10 tracers ; PISCES-noFe-nocarbon : 15 tracers ; PISCES-nocarbon : 21 tracers ; PISCES : 24 tracers ; PISCES (+ additional modules : DMS, N2O, ...) : > 24 tracers …

• coarsening of BGC models: keep a reasonable coast while increasing ocean resolution
  - horizontal coarsening of the outputs (reduction of storage for long runs or tendency terms diagnostic)
  - time and space (horizontal) on-line coarsening of BCG model : can be view as a super-parameterization of the ocean dynamics used for the BGC model ==> much faster BGC component will keeping the benefit from higher ocean resolution (Lévy et al 2012).
• modification of the split between BGC and dynamics
  - BCG model restricted to SMS terms. The transport part (advection/diffusion) should include the sinking of particles, i.e. all terms that depend on the ocean dynamical kernel. As such, the kernel of the BGC model becomes independent from the ocean kernel. In particular, it will be much easier to use PISCES in any other ocean model (structured as well as unstructured one).
  - PISCES SMS can then be rewritten as a 1D problem to act only on unmasked ocean points (less computation). In the 1D vector, ocean point would be order as a function of increasing depth, allowing easy restriction of the computation of some SMS terms (the one being non zero only in the upper ocean or near the ocean floor).
• BCG and sea-ice : see §III on ice
• BCG-land interface :
  - management of carbon and nutrient fluxes provided by land models (use of a generic estuarine model)
• BCG-atmosphere interface :
  - dependency of air-sea BGC fluxes on the sea state (coupling with wave model)
  - dependency of air-sea BGC fluxes on dust deposition (coupling with aerosol model)
  - dependency of ocean surface albedo as a non-linear function of surface winds, surface chlorophyll and solar zenith angle (Jin et al. 2004).
• BGC-ocean interaction in ocean only simulations (short term)
  - RGB case: set a chlorophyll profile from surface ocean colour (Uitz et al.)
  - 2 bands case: use a second band length scale that depends on ocean colour (Murtugudde et al.)
• BGC and paleoclimate: explicit representation of the cycle of tracers used as proxies
• Improved numerics:
  - temporal/spatial scheme : (1) transport part (TRP) follows the evolution of the ocean but constrains this evolution so that TRP can use a larger time step (time coarsening) and has a consistent high order *positive* schemes ; (2) Source minus Sink part (SMS) in PISCES: evaluate alternative schemes for the most constraining SMS terms.

- development of a more efficient algorithm for sedimentation (falling of particles) (lagrangian / semi-lagrangian approach, or time splitting scheme that depends on the size of particles, other?)

III. Ice (Sea-ice & continental ice interface):

III.1 Sea-ice (LIM)

• dynamics:
  - rheology adapted to high resolution (brittle rheology, Girard et al. 2011)
  - Marginal Ice Zone (MIZ): distribution of ice floes, wave-floes interactions
  - fast-land ice in coastal areas

• physics:
  - surface: snow compartment, melt pond
  - open water area : leads and polynia
  - light penetration through snow & ice
  - multi-phase physics and thermodynamics (brines pockets…)
  - ice-ocean interaction: super-parameterization of ocean the mixed layer ; brine rejection ; prognostic bottom ice roughness and ice-ocean stress ; wave-ice interactions
  - ice-air interaction: prognostic surface roughness and ice-air stress ; downscaling of surface forcing

• BGC compartment in sea-ice and its interactions with both ice physics and ocean BGC

• coupled interface for multi-category sea-ice (with atmosphere and wave models)

• share LIM thermodynamics and BGC with any other ocean models
  - ice thermodynamics and BGC SMS re-written independently of the host ocean model (i.e. suitable for structured as well as unstructured one).

• sea-ice interface : addition of the interface with Gelato sea-ice model

• HPC :
  - how improved the scalability of the ice ? Change in the domain decomposition for ice ?
  - use of a coarsening technique for the ice

III.2 interface with ice sheet

• Icebergs (ICB):
  - interface with wave model : waves strongly constrain iceberg trajectories.
  - further improvement : current/iceberg interactions, large tabular iceberg case, thermodynamics (constant versus prognostic iceberg temperature, …)

• Under ice shelf seas (UIS):
  - 1, implement under ice shelf seas using partial step coordinate (zps)
  - 2, introduce mixed zps/sco coordinate in order to better represent the ocean boundary layer below ice shelves
  - 3, introduce the capability of having time varying under ice shelf sea cavities

• coupled interface of ICB and UIS with ice sheet model in an ESM framework

IV. Assimilation interface and tangent & adjoint models

IV.1 Identified actions to be taken at a relatively short time scale:

• observation operator (OBS) :

- This module requires code cleaning and simplification, for instance it should only support its own so-called 'feedback' format for reading the data, and an off-line translator could be provided for the most common datasets.
- The above cleaning is a good opportunity the check if the current observation internal framework is sufficient for dealing with new observations types : ocean (tide gauges, floats, gliders, SWOT…), sea ice (concentration, thickness…), BGC (ocean color, oxygen, nitrate, Iron…), icebergs, ...
- Finally, one should promote the use of this module for model-data inter-comparisons.

• Increment (ASM) :

- increment for sea ice and BGC models
- ensemble run: build-in ensemble of simulations performed in parallel with MPI communication between members of the ensemble to compute on-line statistics.

• Tangent and Adjoint Model (TAM) :

- maintain OPA-TAM phasing and survey of automatic differentiation tools
- The non-linear free-surface is missing in TAM due to the large amount of coding it requires. One should review the choice and check whether the current approximation (direct model with nonlinear free surface, adjoint with linear) is satisfactory or not.
- The mixing coefficient are considered as passive variables in TAM, i.e. constant in the tangent model (computed by the direct model) because mixing schemes such as TKE are known to be unstable in tangent mode. Again, one should review this approximation and if necessary investigate other approximations and/or other mixing schemes.

• environment :

- promote the use of data assimilation techniques (variational and/or stochastic approaches) for operational forecasting, parameter estimation, design of new parameterizations, sensitivity analysis, computation of characteristic vectors (singular vectors, Lyapunov vector, EOFs, ...), etc…
- One or several reference configurations including 3D and 1D mono/multi-component test cases (based on SEABASS for instance) could be proposed for sequential and variational data assimilation and demonstrators (tutorials) illustrating the various potentiality of the system should be provided.

IV.2 Possible path of action that requires investigation prior to implementation

• observation operator (OBS) :

- Investigate the feasibility and potential gain of moving OBS in the I/O server

• Increment (ASM) :

- The possibility to handle increments (or other fields) on different grid resolution at the same time would be useful for both sequential and variational approaches (for multi-grid algorithms).

• Tangent and Adjoint Model (TAM) :

- investigate the need to develop TAM for other components : BGC (Kane et al. JGR2011), sea-ice (Heimbach et al OM 2010). Maybe a good way would be to develop it in 1D and compare it with stochastic filtering alternatives to variational approach.
- Would extend TAM in case of AGRIF grid refinement be useful ?

IV.3 Research topics that may (or may not) lead to implementation in NEMO.

- TAM based tool for initialization?
  - well-balance initial state of regional configurations or AGRIF child
  - transformation of ocean increment produced by sequential methods into a balanced one

V. System environment

- simplify the setting and run of targeted configurations (global, regional or coastal configurations with multiple AGRIF grid refinements) in an ESM framework (*i.e.* up to a ocean/BGC/sea ice/ice sheet/waves/land/atmosphere system)
- integrated system (multi-components) but preserve stand alone capabilities for each part: preserve the physical & numerical upgradability of each individual component
- Extensive code rewriting for consistency, better reliability and performance and improved modularity (is this possible in the next 10 years, or is it a dream?)
- provide a new suite of validated test cases (legacy of COMODO) and tutorials