Technical and physical challenges to achieve a regional simulation at multi-decadal scales: Applications to the Bay of Biscay.

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Objectives

In the framework of the ENIGME project, aiming to study the hydrodynamic variability in the Bay of Biscay and the English Channel over decadal and multidecadal periods, we build and use numerical simulations based on the MARS3D code.

Such numerical experiments led to rise several physical and technical issues. In particular :

- ➔ To have a continuous and coherent atmospheric forcing dataset on a long period,
- ➔ To design the best solution for oceanic forcings,
- ➔ To manage and optimize parallelization computing and input/output strategy in the aim to gain performance on dedicated supercomputer.

Solving these different questions lead to the first 53 year long simulation on the Bay of Biscay and the English Channel (first results in Charria *et al.*,2014 – poster n°B976).

MARS3D model presentation

MARS 3D Equation system (Duhaut *et al.*, 2008, Lazure *et al.*, 2005) is based on geophysical fluid dynamics: **primitive equation with a free surface to represent the gravity waves in the coastal area.**

The sigma coordinate is used on the vertical dimension to resolve simultaneously the shallow and deep water column.

The main code equations are :

Momentum equations :

$$\frac{\partial u}{\partial t} + L(u) - fv = -g\frac{\partial \zeta}{\partial x} - \frac{1}{\rho_0}\frac{\partial p_a}{\partial x} + \Pi_x + \frac{1}{\rho_0 H_z}\frac{\partial \tau_{xz}}{\partial \sigma} + \mathcal{F}_x$$

$$\frac{\partial v}{\partial t} + L(v) + fu = -g\frac{\partial \zeta}{\partial y} - \frac{1}{\rho_0}\frac{\partial p_a}{\partial y} + \Pi_y + \frac{1}{\rho_0 H_z}\frac{\partial \tau_{yz}}{\partial \sigma} + \mathcal{F}_y$$

$$\frac{1}{H_z}\frac{\partial p}{\partial \sigma} = -\rho g$$

$$\frac{\partial \zeta}{\partial t} + \frac{\partial (H_z u)}{\partial x} + \frac{\partial (H_z v)}{\partial y} + \frac{\partial (H_z \tilde{w})}{\partial \sigma} = h\phi$$

where :

$$L(A) = u\frac{\partial A}{\partial x} + v\frac{\partial A}{\partial y} + \tilde{w}\frac{\partial A}{\partial \sigma}$$

$$\Pi_x = \left(\frac{\partial}{\partial x}\right)_\sigma \left[\int_\sigma^0 H_z b d\sigma'\right] - b\left(\frac{\partial z}{\partial x}\right)_\sigma$$

$(\sigma = 0)$.

$$\Pi_y = \left(\frac{\partial}{\partial y}\right)_\sigma \left[\int_\sigma^0 H_z b d\sigma'\right] - b\left(\frac{\partial z}{\partial y}\right)_\sigma$$

Tracer equation : temperature and salinity

In the σ coordinates, for a consistant *c*, the MARS model solves the following equation :

$$\frac{\partial (H_z c)}{\partial t} + \frac{\partial}{\partial x}\left[H_z\left(uc - \kappa_H\frac{\partial c}{\partial x}\right)\right] + \frac{\partial}{\partial y}\left[H_z\left(vc - \kappa_H\frac{\partial c}{\partial y}\right)\right] + \frac{\partial}{\partial \sigma}\left[H_z(\tilde{w}c)\right] - \frac{1}{H_z}\frac{\partial}{\partial \sigma}\left(\frac{\kappa_V}{H_z}\frac{\partial c}{\partial \sigma}\right) = H_z(s^c - p^c)$$

The fast external motions can be modelled accurately with a two-dimensional barotropic subsystem dealing with the shallow water equations for a homogeneous fluid (finite difference scheme with ADI Alternating Direction Implicit method on the Arakawa C grid). The remaining slow motions can be modelled by a three-dimensional baroclinic subsystem. The barotropic and baroclinic mode are the same time step. The new numerical MARS code can run without explicit viscosity.

BACH4000 configuration

Code version	MARS3D V10
Resolution	4 km / 40 levels
Domain / period	41°N – 52.5°N / -15°W – 4°E - 1958 to 2010
Vertical coordinates	Generalized sigma coordinates
Bathymetry	Composite
Runoff	95 Rivers
Tides	Disabled for the first long term simulation
Vertical mixing	k-epsilon (Rodi *et al.*, 1993)
Atmospheric forcing	ERA-40 (1958-1978) and ERA-Interim (1979-2010)
Oceanic forcing	• Global model ORCA025-GRD100 (NEMO model based) in hindcast mode at open boundaries (temperature, salinity, sea surface height, barotropic and baroclinic velocities) • Tides : FES2004 harmonic composition (if enabled)
Initial condition	• Global model ORCA025-GRD100 (NEMO model based) in hindcast mode (temperature, salinity, sea surface height, barotropic and baroclinic velocities)
Bottom friction	Quadratic bottom friction (Z_0 formulation)
Bulk formulation	Solar flux (Gill, 1982) Infrared flux (Swimbank – EDF, Agoumi thesis) Turbulent fluxes: - Clark *et al.* (1995) – latent flux + modifications - Elliot and Clark (1990) – sensible flux + modifications
Viscosity	Implicit

Atmospheric and oceanic forcing

Atmospheric forcing

To perform a long term regional simulation, we need coherent long term atmospheric forcing covering the whole period (1958-2010). The most efficient approach would be to use the same forcings used in the global simulation (Drakkar Forcing Set – DFS - for the ORCA025-GRD100 simulation – table 2). However, some variables are missing (cloud coverage) due to our bulk formulation in MARS3D. Then, we investigate the use of ECMWF (European Centre for Medium-Range Weather Forecasts) for reanalyses (ERA-40 and ERA-Interim – table 1).

Characteristics	ERA-40	ERA-Interim
Domain	Global	Global
Spatial resolution	1.25°	0.75°
Temporal frequency	6 hours	6 hours
Period	Sept. 1957 – Aug. 2002	Jan. 1979 – Dec. 2010

Table 1: Description of ECMWF reanalyses.

The periods covered by ERA-40 and ERA-Interim are overlapping for the years between 1979 to 2002. Following the improvements in the most recent ERA-Interim reanalysis, we give priority to this product for the most recent years. The atmospheric forcing scenario is represented in the figure 1.

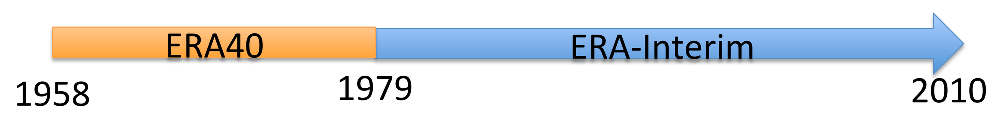

Fig. 1: Time line for atmospheric forcings in BACH4000 configuration.

The coherency between the Drakkar Forcing Sets used in the global simulation (the ORCA025-GRD100) and the ERA reanalyses has been evaluated. For example, in figure 2, the net heat fluxes are similar for our region in both datasets. Indeed, DFS5 are based on the same reanalysis but it has been adjusted at global scale (Brodeau *et al.*, 2010). These results validate the approach.

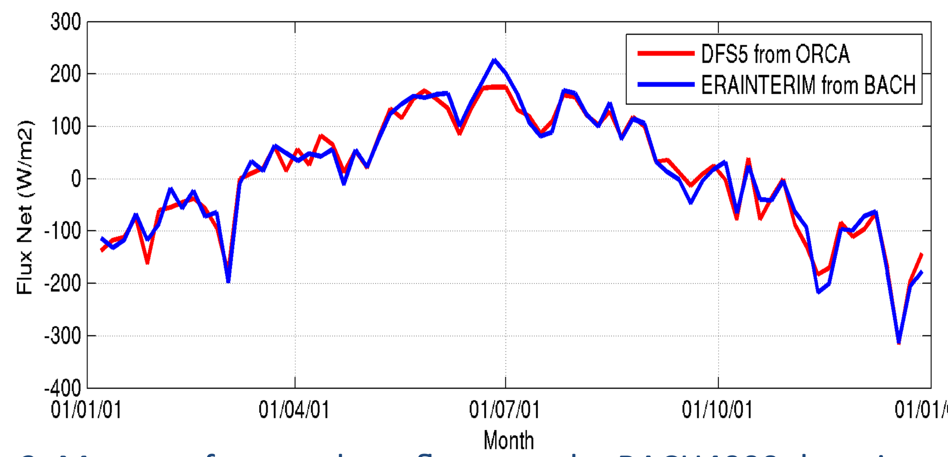

Fig. 2: Mean surface net heat flux over the BACH4000 domain.

Oceanic forcing

Ocean forcings are based on a global simulation (ORCA025-GRD100 – table 2) performed in the frame of the DRAKKAR project and covering the whole period for our regional application.

Characteristic	ORCA025-GRD100
Domain	global
Horizontal spatial resolution	¼°
Vertical resolution (z-coordinates)	75 levels
Period	1958-2010
Atmospheric forcing Brodeau *et al.* (2010)	DFS4.3(1958-1988) DFS5(1989-2010)

Table 2: Overview of the global ORCA025-GRD100 simulation.

These global fields are used for ocean open boundary conditions. Dirichlet conditions are used and combined with a 40km (10 grid points) sponge layer. In this layer, the viscosity and the dissipation are fixed to 10m² s^{-1} and decreases to 0 at the limit of the sponge layer. A strong relaxation coefficient is also applied in this sponge layer with a value of 10 days. Some sensitivity experiments have been performed using different schemes for OBC, but they are not fully efficient for our experiment.

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Technical issues

Simulation framework

For this project, interannual simulations are covering a **53 year period** (1958-2010) with sensitivity experiments based on the last decade.

This long term experiment is producing **daily fields** (2D and 3D variables) and the computation has been performed at CINES on a SGI machine. The numerical cost is related to the grid size (353x560x40 grid points) and input/output strategy. For example, a 53 year simulation costs about **200,000 hours (CPU time)** runnning in 2 weeks and produces about **5 To** (daily outputs). Consequently, a strategy of automatic and regular **restart** has been implemented.

The long computing time for the simulation (50 years) over high resolution grids and producing a large amount of data to be written online imply to solve two main technical issues:

- ➔ Optimization of the domain decomposition and the use of the parallelization,
- ➔ Management of Inputs/Outputs (I/O) through the use of a dedicated I/O server.

Parallelization

We used a grid division tool (Molines, 2004) to perform a domain decomposition avoiding land region and to minimize the number of cells. Each subdomain is then computed on a node composed of 8 cores. Communication between nodes is made possible using MPI and the OPENMP parallelization is used inside each node (figure 3).

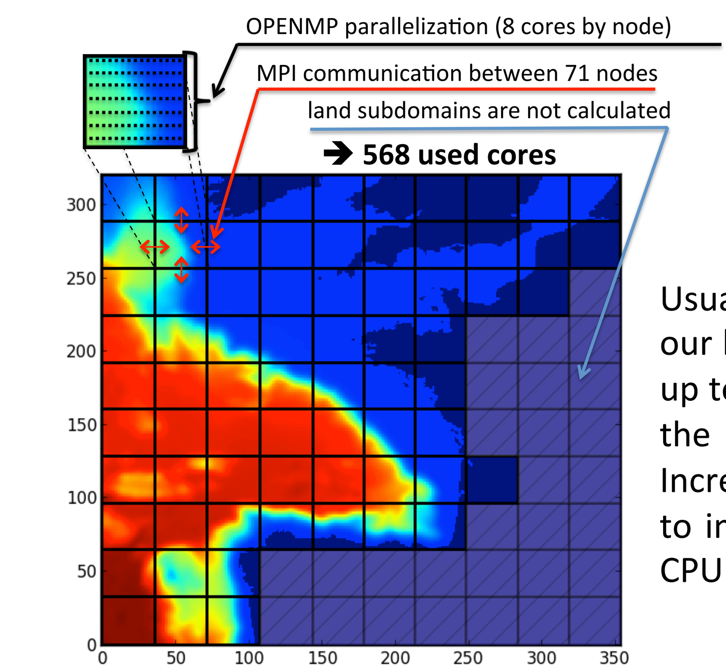

Fig . 3 Domain decomposition used in hybrid mode parallelization (MPI + OPENMP) on 568 cores.

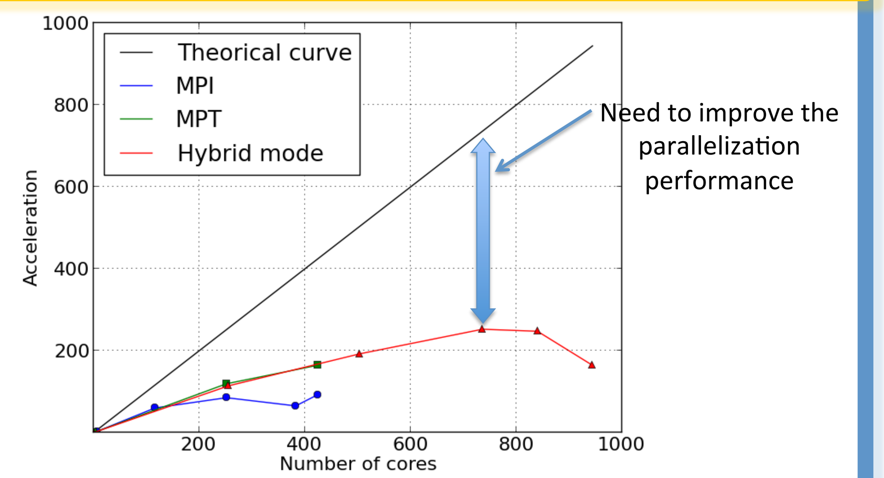

Fig. 4 Acceleration of the BACH4000 configuration on Harpertown cores. (MPT is the MPI implementation on the used cluster). No outputs have been saved for these tests.

Usually a maximum of 256 cores is used for the short term MARS3D simulation. In the case of our long experiment, we have tested several decompositions playing with the number of cores up to about 1000. As seen in figure 4, the use of hybrid mode parallelization (OPENMP + MPI) is the most efficient parallelization mode in our case with respect to the only use of MPI. Increasing the number of cores allows to gain performance but developments have to be driven to improve the performances. In the aim to get a reasonable balance between wall time and CPU time, we select a 568 cores configuration.

Input/output management

The parallel writing of NetCDF4/HDF5 outputs on the Lustre file system with the MARS3D code library shows a large variability in the writing time on the production computer (figure 5). It induces a drastic increase of the cost in terms of CPU time not due to the computation.

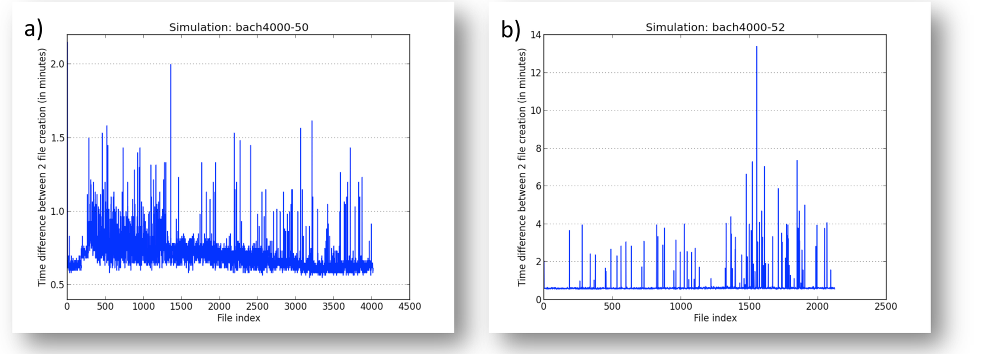

Fig . 5. Two examples of time differences between written outputs. a) and b) are the same simulation, which run at different time. a) Mean time is about 0.7 seconds with peaks at 2 minutes; b) some peaks above 10 minutes inducing the stop of the simulation.

A solution to bypass this I/O problem is to use a dedicated I/O server supporting the load of penalizing writing tasks. Then, the client time computation is not affected by writing. We explored the implementation process and the use of the tool XIOS developed in IPSL (Institut Pierre Simon Laplace) by Y. Meurdesoif *et al.* (figure 6).

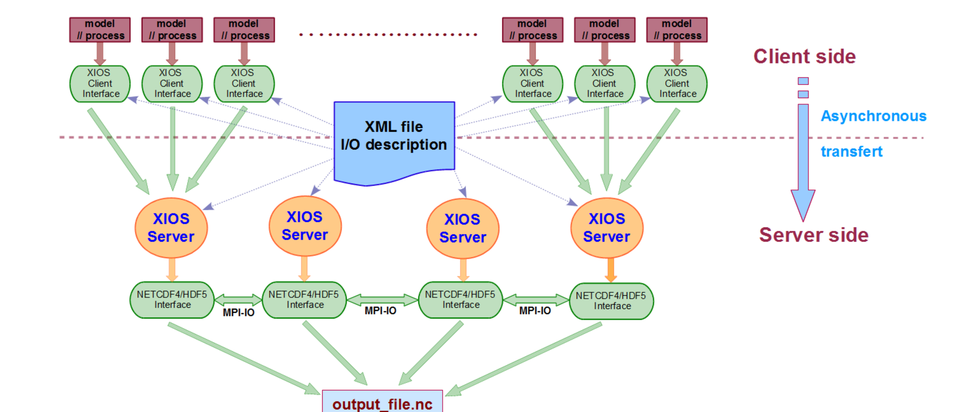

Fig . 6 Description of XIOS (Xml-IO-Server). Computing cores send fields to dedicated writing cores (server mode) and allow simple computation for outputs (*e.g.* averages).

The XIOS server has been implemented in a simplified test case (Kelvin wave on a 52x31x10 grid points – figure 7). We tested this configuration using 3 options : MARS I/O library, XIOS library (online mode) and XIOS server (dedicated cores). The three solutions gave the same results (XIOS works on the target machine !). First results show that the XIOS library is faster (> 3 times) than the original MARS3D I/O library. In the server mode the gain in performance can't be evaluated on simplified test cases but is expected for realistic simulations.

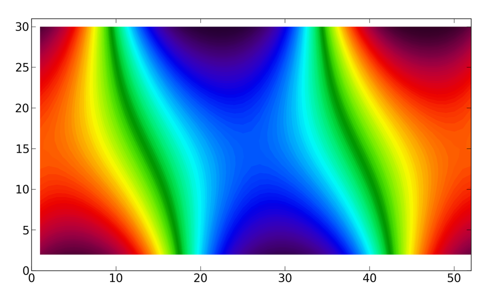

Fig . 7 Sea Surface Height for a propagating Kelvin wave using XIOS in server mode (32 cores for the model computation; 8 cores for writing data).

Conclusions

The present work details physical and technical issues that we had to explore before launching a multi-decadal numerical experiment.

Homogeneous atmospheric forcings on a 50 year period are not available to drive a regional high resolution experiment (4 km). Based on the global simulation forcings (DFS), we validated the use of ECMWF (ERA-40 and ERA-Interim) reanalyses. At open boundary conditions, a first approach has been designed related to the ORCA025-GRD100 simulation but needs to be improved (*e.g.* to implement a convergence in the sponge layer between global and regional bathymetries, to reduce the relaxation constrain).

For the two main technical issues (parallelization and I/O strategy) an optimal design is implementing. The hybrid MPI/OMP parallelization mode has been selected associated to the most performing domain decomposition (further investigations are in progress in collaboration with CINES technical group on the library environment). The use of XIOS dedicated server appears as a promising solution for I/O issues associated with an extended flexibility for writing outputs.

Based on these investigations, future experiments will be possible and designed (*e.g.* higher resolution).