Towards a 3D Hydrodynamic numerical modeling system for long term simulations of the Río de la Plata dynamic

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ABSTRACT

In order to support water management decisions involving characteristics of the Río de la Plata current fields, a 3D hydrodynamic baroclinic numerical model has been implemented. Firstly, a 2D South Atlantic hydrodynamic barotropic model forced by NCEP reanalysis winds and the astronomical model FES2004, called 'AStide' is implemented and calibrated, taking the quality in the representation of the water level oscillations at the mouth of the Río de la Plata as the calibration condition. Secondly, a 3D hydrodynamic baroclinic model, with ten vertical sigma layers, forced for fluvial discharges, ECWMF reanalysis winds and boundary conditions from the AStide model, called 'RPtide' is implemented and calibrated. The computational tool used for the simulations is based on the MOHID water system and was developed with the aim of achieving a good quality in the dynamic representation while maintaining independence in the execution and efficient computation times. In order to improve the performance of the tool, several HPC techniques were applied, achieving speedups of up to 2x, while further improvements on the computational schemes used in the model allowed a 25% reduction in the running time. The proposed tool was used and validated, based on a hindcast strategy using the MOHID water system, in the evaluation of the potential energy of tidal currents in the area..

Keywords: hydrodynamic modeling, high performance computing,

1. INTRODUCTION

The Río de la Plata is a complex water body with fluvial–estuarine characteristics located between Argentina and Uruguay (34°00'–36°10' South and 55°00'–58° 10' West). On its margins are located the capital cities of both countries, Buenos Aires and Montevideo respectively, the principal harbors of each country and several industrial and touristic centers. Therefore the Río de la Plata hydrodynamics play an important role in both economic and social aspects being responsible for catastrophic floods in many coastal areas and controlling the fluvio-maritime traffic.

In order to support water management decisions involving characteristics of the Río de la Plata current fields, a 3D hydrodynamic baroclinic numerical model has been implemented. Further, considering that the meteorological tide in the Río de la Plata, mainly resulting from the atmospheric processes acting over the continental platform and over the adjacent oceanic region, represents the 50% of the tidal energy (Santoro et al, 2013) a nested system is then defined. The model system is based in previous hydrodynamics models implemented in the zone with the MOHID code (Santoro et al, 2011; Fossati et al, 2013).

The computational tool used for the simulations is based on the MOHID water system (Mateus and Neves, 2013) and was developed with the aim of achieving a good quality in the dynamic representation while maintaining independence in the execution and efficient computation times. MOHID presents an integrated modeling philosophy, not only of processes (physical and biogeochemical), but also of different scales (allowing the use of nested models) and systems (estuaries and watersheds). The MOHID model is considered to be one of the most elaborate models of this type for its conception, reliable and robust framework, as well as for its diversity of vertical coordinates. MOHID encompasses a standard finite-volume approach of the Ocean Primitive Equations, using a generic combination of sigma and/or Cartesian vertical coordinates with an ADI semi-implicit scheme for the horizontal advection–diffusion numerical schemes, as well as possessing a complete suite of modern and standard open boundary conditions.

Firstly, a 2D South Atlantic hydrodynamic barotropic model forced by NCEP reanalysis winds and the astronomical model FES2004, called 'AStide' is implemented and calibrated, taking the quality in the representation of the water level oscillations at the mouth of the Río de la Plata as the calibration condition. Secondly, a 3D hydrodynamic baroclinic model, with ten vertical sigma layers, forced for fluvial discharges, ECWMF reanalysis winds and boundary conditions from the AStide model, called 'RPtide' is implemented and calibrated.

In order to use the modeling system in the evaluation of the potential energy of tidal currents in the area long term simulations of several years were needed. Then the performance of both models was improved applying several HPC techniques.

The aim of this article is to present the advances in the development of a model system for long term hydrodynamic simulations of the Río de la Plata and the Uruguayan coast. This paper is organized in three main sections. The first one describes the characteristics and the calibration process for the 2D model. The second one present the main aspects related with the 3D model. The third one describes the methodology used for the computational performance improvement, and the application of HPC techniques. Finally, the article concludes with some final considerations and lines of future research.

2. 2D AStide model

2.1 Implementation

The AStide model solves the bidimensional flow in the South Atlantic Ocean in the domain [22ºS; 54.4ºS]-[70ºW; 45.5ºW] (Figure 1). The mesh has a latitude-longitude structure with a constant discretization of 0.1º. The bathymetry of the area was generated from GEBCO and other regional bathymetry data. Finally, the line coast of the area was built from NOAA/NGDC Marine Geology and Geophysics Division database.

The open boundary condition is used to impose the astronomical tide effect into the calculation domain. The water level is calculated every two cells of the oceanic border from the superposition of 13 tidal harmonic constituents obtained from the FES2004 model (Lyard et al., 2006). In addition to that, the Blumberg & Kantha relaxation scheme is implemented as boundary condition using 100 seconds lag time in deep water and 100 seconds in shallow water with a linear variation in the transition zone (Blumberg & Kantha, 1985). Null velocities and a 0,91m mean water level were imposed as model initial conditions. Finally, reanalysis of 6 hours temporal resolution and 0.5º spatial resolution from National Centers for Environmental Prediction (NCEP) of USA (Saha et al., 2010) was incorporated as the atmospheric forcing on free surface.

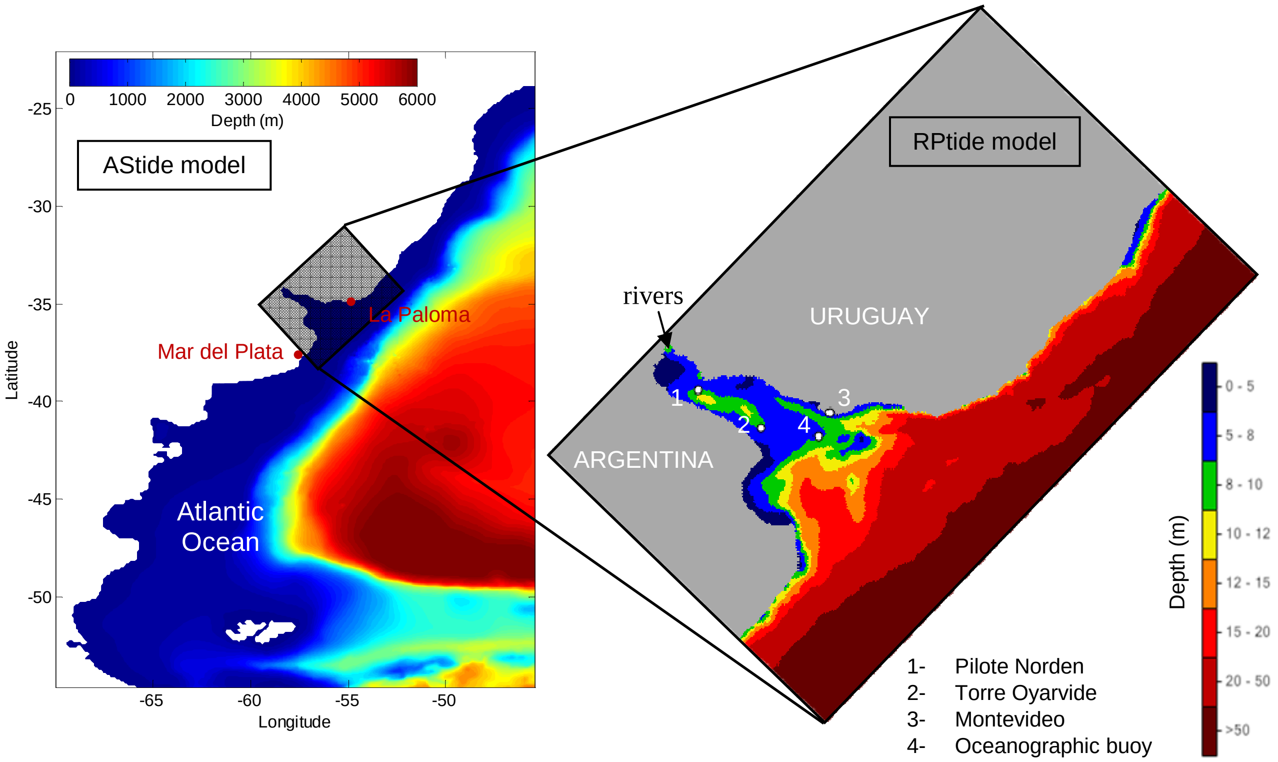

Figure 1. AStide and RPtide model domain and bathymetry.

2.2 Calibration

The calibration methodology consists in performing different short test simulations changing one of the calibration parameters involved in the main processes in each of the simulations. The specific parameters that were switched are the wind drag coefficient (Cd), the friction coefficient in the bottom (n), the influence of atmospheric pressure, the turbulence parametrization, the oceanic boundary condition, and the time step. Thus, the sensitivity of the model was determined against each of the parameters changes. The selected period to execute the test simulations is March 2004. Once all test simulations were executed, the results are compared with hourly water level time series recorded during the simulated period in two stations located in the mouth of the Rio de la Plata (Mar del Plata and La Paloma, see location in Figure 1). An error analysis of each test simulation was performed by using three statistical indicators: the root mean square error (RMSE, Eq. [1]), the relative RMSE (RMSE divided by the mean amplitude), and the correlation coefficient (R, Eq. [2]); where x_i and y_i are the observed and modeled variables, respectively and N is the number of measurements in the time series.

$$RMSE = \sqrt{\frac{1}{N}\sum_{1}^{N}[(x_i) - (y_i)]^2}$$

[1]

$$R = \frac{\frac{1}{N}\sum_{1}^{N}(x_i - \bar{x})(y_i - \bar{y})}{\sigma_x \sigma_y}$$

[2]

In order to select the best model parametrization, the resulting water level errors were analyzed using Taylor diagrams and the influence of each parameter on the water level results was considered. Afterwards, model stage validation was performed by simulating the years 2003 and 2004 with the chosen configuration, where statistical indicators mentioned above were calculated and errors were visualized in Taylor diagrams. Finally, the tidal harmonic constituents computed from model time series and measurements were compared.

2.3 Results

The parameters that have the highest influence on the water level results are firstly the drag coefficient of wind and secondly the consideration or not of atmospheric pressure. The turbulence parametrization and the relaxation condition at open boundaries have almost no influence over water level series at the Río de la Plata.

The selected configuration has the following main characteristics: no consideration of atmospheric pressure, Large & Ponds formulation to calculate drag coefficient of wind, Manning number of 0.005 at the bottom, Blumberg & Kantha relaxation scheme at the open boundaries with a lag time of 100/1000s, and Smagorinsky formulation with coefficient of 0.1 to calculate the turbulent horizontal viscosity.

The water level mean errors, quantified as RMSE, are 0.22 m in Mar del Plata and 0.21 m in La Paloma. This represents a mean error reduction of 15% and 22% in Mar del Plata and La Paloma respectively, compared with the non-calibrated AStide configuration. The high quality of data fit can be seen in Figure 2, where comparisons of water level time series of Mar del Plata and La Paloma are shown. The fit errors of tidal harmonic constituents are shown in Figure 3 and 4 as Taylor diagrams, where the errors parameters of the simulated series are visualized and compared with measurements. At Mar del Plata, where astronomical tide predominates, the main constituents (M2, K1, S2, O1, and N2) are placed very near of measurements because of the high quality fit. At La Paloma, where metereological tide predominates, the quality fit decreases.

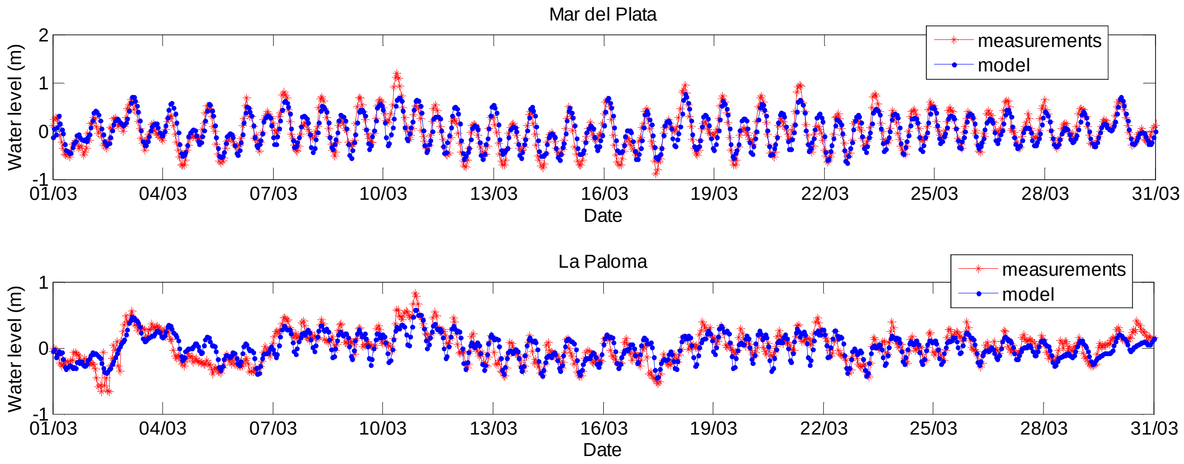

Figure 2. Time series comparisons between measured and simulated water level at Mar del Plata (up) and La Paloma (down).

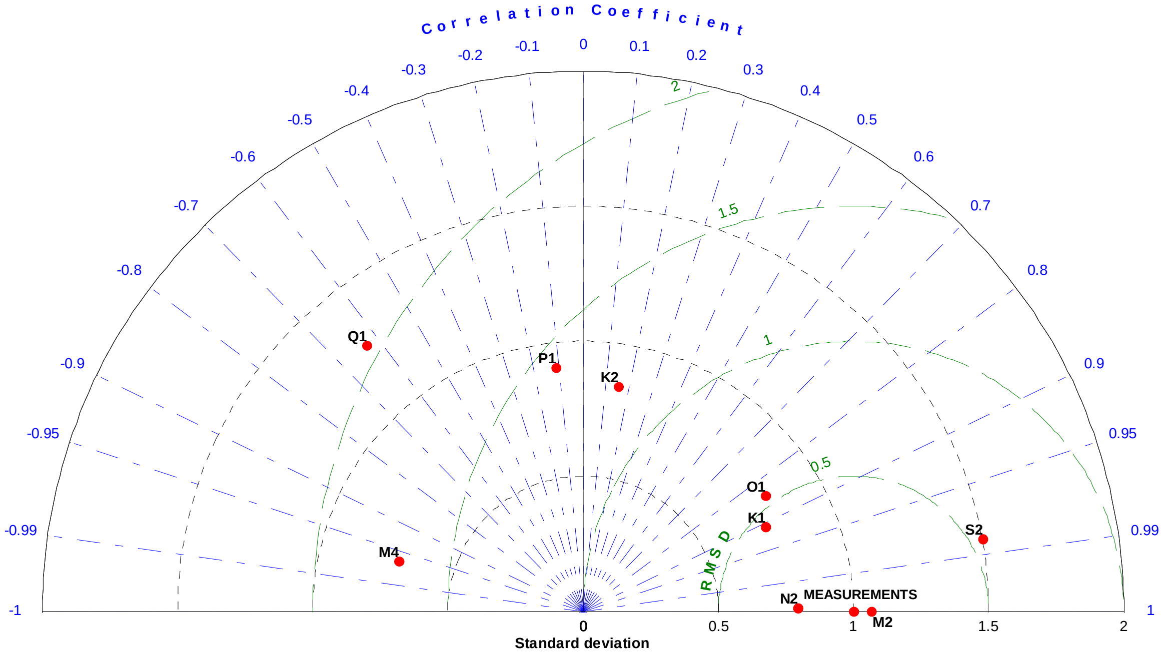

Figure 3. Taylor diagram of measured and simulated tidal harmonic constituents at Mar del Plata

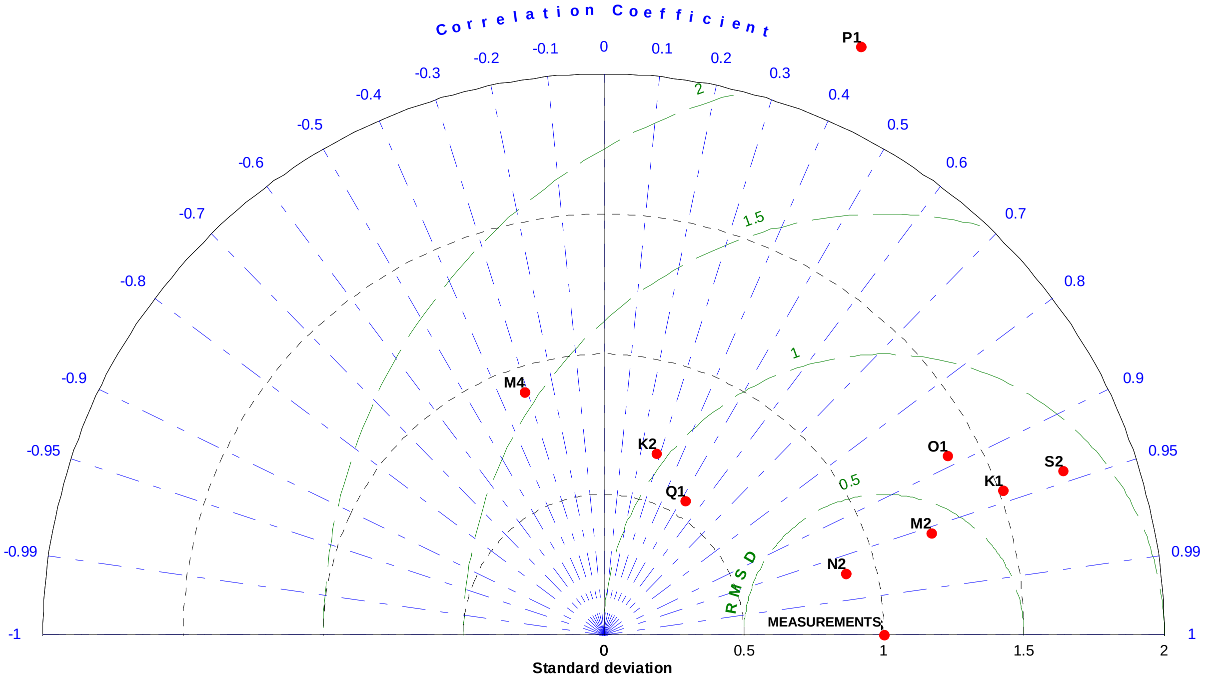

Figure 4. Taylor diagram of measured and simulated tidal harmonic constituents at La Paloma

3. 3D RPtide model

3.1 Implementation

The 3D hydrodynamic baroclinic numerical model of the Rio de la Plata called RPtide is currently being developed. This model is forced by the resulting data of AStide model at oceanic boundaries, by high-resolution winds on the surface obtained from the global database ECMWF (European Centre for Medium Range Weather Forecast) (Dee, et al., 2011) with a spatial resolution of 0.25º and a temporal resolution of 6 hours, and by the flow contribution from Uruguay, Parana-Las Palmas and Parana-Guazú rivers.

The RPtide domain (Figure 1) comprises between the Río de la Plata head where the rivers discharge until the area bounded between Mar del Plata (Argentina) and Rio Grande (Brazil) extending approximately 170km offshore. The bathymetry of the area was elaborated from the Uruguayan Oceanographic, Hydrographic and Meteorology Service of the

Army (SOHMA) and the Argentinian Naval Hydrographic Service (SHN) databases. The line coast was built from NOAA/NGDC Marine Geology and Geophysics Division database and from local high-resolution measurements. The three-dimensional mesh has a latitude-longitude structure, constant horizontal discretization of 0.02º, and 10 vertical layers defined from sigma coordinates using constant coefficient.

3.2 Calibration

The RPtide calibration methodology consists in the performing of different test simulations where in each one a calibration parameter of the model is changed. The boundary conditions imposed on the water border, the drag coefficient of wind at the surface, the friction coefficient in the bottom, and the turbulence parametrization were the selected calibration parameters. The test simulation results were compared with water level and salinity time series measured at Pilote Norden, Torre Oyarvide, and at an oceanographic buoy (see locations in Figure 1) during the FREPLATA/FFEM Project (FREPLATA, 2011). The selected period to execute the test simulations is July 2010. Pilote Norden and Torre Oyarvide are fixed mareographic stations placed in the interior and intermediate zone of Río de la Plata, respectively. Both stations have installed a SMATCH equipment that records water temperature, conductivity, turbidity, and depth (FREPLATA, 2004) at 3 m from surface. This equipment measures in an absolute reference respect to movement of sea. The oceanographic buoy is a floating element on the water surface placed in the intermediate zone of Río de la Plata and anchored to two cinderblocks with the objective of remaining in the same site. The buoy has installed a SMATCH equipment which is located 2.5m below the free surface.

In order to evaluate the quality of the model results, graphic representations of simulated and measured time series of water level and salinity were made, as well as salinity vertical profiles and visualizations of the residual velocity fields. The error of the representation was quantified by the definition of the same two statistical indicators mentioned before: the RMSE and the correlation coefficient (R).

3.3 Results

The selected configuration has the following main characteristics: consideration of atmospheric pressure, Large & Ponds formulation to calculate drag coefficient of wind, drag coefficient of 0.00065 at the bottom, Blumberg & Kantha relaxation scheme at the open boundaries with a lag time of 1000s, Smagorinsky formulation with coefficient of 0.4 to calculate the turbulent horizontal viscosity, and General Ocean Turbulence Model (GOTM) to model vertical turbulence (included in MOHID code).

At Pilote Norden the water level RMSE error obtained is 0.34 m and presents a correlation coefficient of 0.69. At Torre Oyarvide the water level RMSE is 0.24 m and the correlation coefficient is 0.85, while the salinity RMSE and correlation coefficient is of 0.40 ppt and 0.29 respectively. At the oceanographic buoy the RMSE obtained is 3.39 ppt and the correlation coefficient is 0.73. The comparisons of measured and simulated time series of water level at Pilote Norden and Torre Oyarvide are shown at Figure 5, observing a high quality fit. Furthermore, the salinity time series and vertical profiles at the oceanographic buoy are presented in Figure 6. The salinity profile shows the different periods of mixing or stratification profile characteristic of the estuarine Río de la Plata zone.

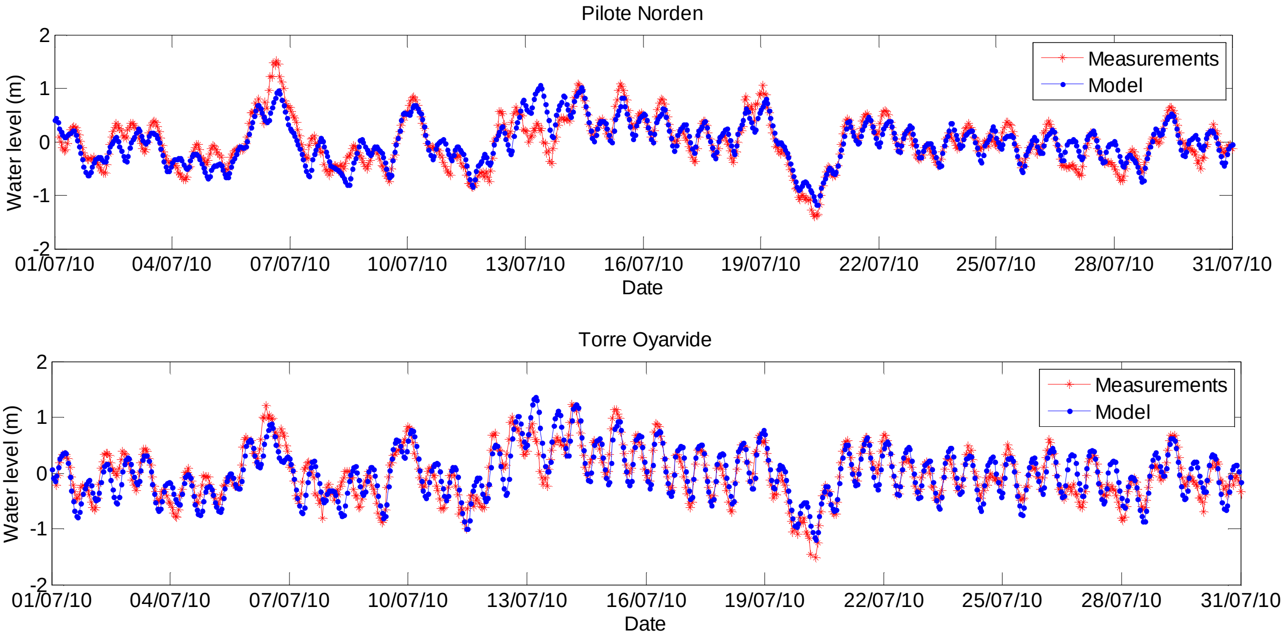

Figure 5. Time series comparisons between measured and simulated water level at Pilote Norden (up) and Torre Oyarvide (down).

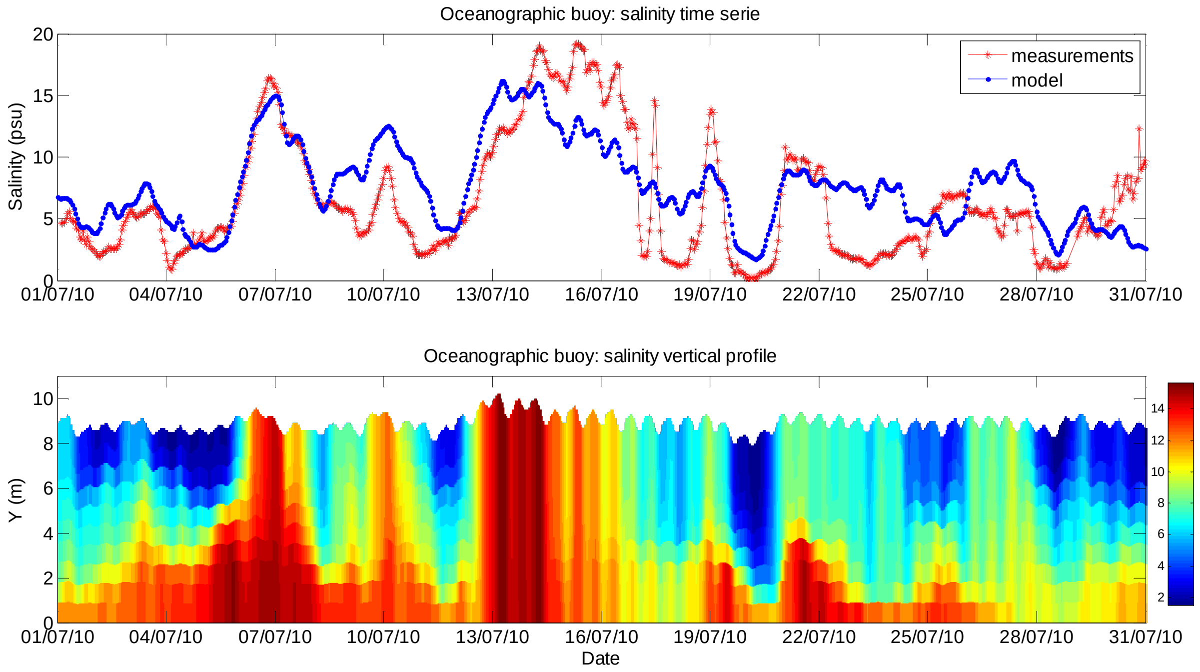

Figure 6. Time series comparisons between measured and simulated salinity (up) and salinity vertical profile (down) at the oceanographic buoy.

The residual velocity fields at bottom and surface are presented in Figure 7. The results show a bottom general circulation dominated by the fluvial outflow discharge at the inner Río de la Plata zone, and dominated by up-river currents in the deeper areas at the outside part of the Río de la Plata. The salty water enters from the Atlantic Ocean through the bottom of the estuary head mainly by the Uruguayan coast. The resulting circulation through the boundaries is on SW-NE direction, that is entering from SW border and outcoming through NE border, while the circulation through open ocean border is almost null.

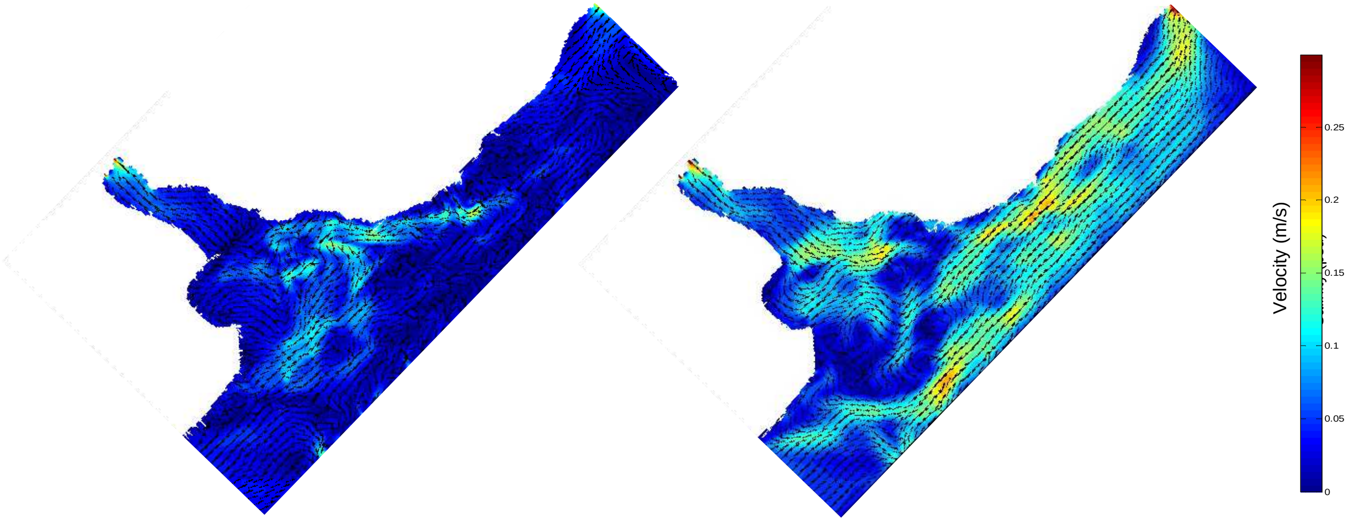

Figure 7. Residual velocity fields of RPtide model at layer 2 (left) and layer 9 (rigth), period July 2010.

4. COMPUTATIONAL PERFORMANCE

As we stated previously, these are powerful models that allow simulating many features and hydrodynamic properties. However, one of the main drawbacks of these models is the large amount of time required to perform simulations for realistic scenarios. In this line, an empirical approach is used to determine which routines represent the main bottlenecks regarding execution time. Then, our effort is concentrated on diminishing the computational weight of these functions. Our research group has successfully applied this methodology to other numerical models for fluid dynamics, such as the RMA-family (Ezzatti et al., 2011), the Caffa 3D (Igounet et al., 2012); and for a weather forecasting model (Silva et al. 2014).

4.1 Profiling

The experimental evaluation was performed in one node of the ClusterFing (www.fing.edu.uy/cluster), particularly in a platform consisting of two INTEL Xeon OctaCore E5-2650 processors (2.00GHz) with 32GB of memory. We use the INTEL compilers version 14 over CentOS as a distribution of Linux OS.

The test cases used in the experimental evaluation were obtained from representative scenarios of 3 months and 7 days for the AStide and RPtide models respectively. The AStide has 42417 active cells and the oceanic boundary condition is imposed in 254 boundary cells. Water level and the two bidimensional velocity components are the model variables. The RPtide model has 38,807 horizontal active cells with 10 vertical layers each. At the oceanic boundary, the water level coming from the AStide model is imposed in 330 cells. Water level and the two velocity components and salinity in each vertical layer are the model variables.

The simulation for the test case of the Astide model implied more than 68600 seconds of execution time, of which nearly 80% corresponds to three routines: Modify_OpenBoundary (69%), ModifyMatrixesOutput (5%) and AdvectionDiffusionIteration_1 (4%).

In the case of the RPtide model, the total runtime is approximately 20900 seconds, 60% of which is concentrated in only three routines: Modify_OpenBoundary (31%), ModifyMatrixesOutput (17%) and TurbGOTM (13%).

4.2 Proposal

In a first stage we focused our efforts only in the routines Modify_OpenBoundary and ModifyMatrixesOutput as they represent an important fraction of the total execution time of both models.

4.2.1 Modify_OpenBoundary routine

This routine is responsible for imposing the boundary conditions on the open borders, and it is invoked at least 10,000,000 times in the AStide model and 1,000,000 times for the RPtide model, for our test cases.

From an algorithmic viewpoint, the routine is composed mainly by four loop sentences that iterate through all the points of the grid. These instructions are parallelized by OpenMP clauses. Two loops show negligible runtimes and the other two spend most of the time performing calls to the routines GetIJWaterLevel and GetIJReferenceLevel. In turn, these two routines present a computational bottleneck on the use of the GetXYCellZ function.

The GetXYCellZ routine takes the position (x,y) of a particle and one specific domain and returns the cell where it is located. The routine operative strongly depends on the kind of grid employed, and dramatically differs according to what kind of step is used (e.g. uniform, variable, constant or uniform rotated). In the case of square cells in the boundary (BorderType), the first column and first row of the grid are used to search the position (x,y). In the original version, both structures (the first column and first row) are copied to an auxiliary data structure. The auxiliary data is dynamically allocated and, even though this is a reduced memory space, this operation is performed a large number of times throughout the simulation (more than 10,000,000 times in the AStide case).

An initial modification consisted in allocating a memory space to hold the auxiliary data structure only one time at the beginning of the execution, as we determined that the upper and lower bound for this structure remains unchanged in the entire simulation. In a second stage, we slightly modified the data structures to avoid the use of this auxiliary data. With this modification, we completely remove the costs associated to the auxiliary data allocations (and deallocations) in the GetXYCellZ routine.

4.2.2 ModifyMAtrixOutput routine

This routine is invoked from the main routine of the Hydrodynamic module, and its purpose is the update of several output values.

In algorithmic terms, the routine includes three loops, which are responsible for the update of several 3D structures. Although two of these loops are parallelized by OpenMP clauses, the most computationally expensive of the three (related to the update of velocity values of each point of the grid) is executed in a serial manner.

Taking this situation into account, we first modified the code to diminish the data dependencies between different iterations of this loop, and later, we included the corresponding OpenMP directives to parallelize this section of the code.

4.3 Experimental evaluation

To perform the experimental evaluation of the proposal we employed the same hardware platform as in profiling stage, see Section 4.1.

Tables 1 and 2 present the execution times (in seconds) for the original and the proposed version of the routines Modify_OpenBoundary and ModifyMatrixesOutput, as well as the acceleration factor obtained when using the new version of the code on the AStide and RPtide models respectively The acceleration factor values are simply computed as the quotient between the execution times of the original-version and novel-version of each routine.

Table 1. Runtime (in seconds) of original and proposed version of Modify_OpenBoundary and ModifyMatrixesOutput routines in the AStide model.

	ORIGINAL VERSION	PROPOSED VERSION	ACCEL. FACT.
Modify_OpenBoundary	47,508	3,619	13.1
ModifyMatrixesOutput	3,365	1,276	2.6

Table 2. Runtime (in seconds) of original and proposed version of Modify_OpenBoundary and ModifyMatrixesOutput routines in the RPtide model.

	ORIGINAL VERSION	PROPOSED VERSION	ACCEL. FACT.
Modify_OpenBoundary	6,526	344	18.9
ModifyMatrixesOutput	3,465	992	3.5

The Table 1 and 2 results show significant acceleration factors for all cases. In particular, the new versions outperform the original versions with a factor of 2.6 times for ModifyMatrixesOutput in Astide, and 18.9 times for Modify_OpenBoundary in RPtide. Additionally, in both cases the acceleration factors reached in the RPtide model are larger than the ones obtained for the AStide model. However, the percentage of both routines in the whole runtime of the original RPtide model is lower.

The previous experimental evaluation has shown that significant improvements on the computational efficiency of both routines on both models are attainable when using the proposed version. So, the next step is to evaluate the impact on the performance of the whole models when the modified routines are employed. Table 3 shows the runtime (in seconds) of AStide and RPtide models when the original routines (Original AS/RPtide) and proposed routines (Modified AS/RPtide) are used; as well as the acceleration factor reached on each model.

Table 3. Runtime (in seconds) of original and modified version of RPtide and AStide models.

	ORIGINAL VERSION	MODIFIED VERSION	ACCEL. FACT.
AStide	68,680	22,917	3.0
RPtide	20,903	12,322	1.7

The results in Table 3 show that important acceleration factor values can be obtained when using the new routines, specifically values of 1.7 for RPtide and 3.0 for AStide case. It should be note that we address the 48% and 74% of the total runtime in the RPtide and AStide respectively. These results are strong consistent with the percentage of each tool that are covered in our effort.

5. CONCLUSIONS

A three-dimensional hydrodynamic modeling system for large simulations of several years for the Río de la Plata water body has been developed. The developed tool consists of a group of integrated models. Although the area of interest is the Río de la Plata region, the system of models needs to be implemented in a bigger domain that includes a large area of the South Atlantic Ocean (AStide model) and then, using the nesting approach, the model focuses on the Río de la Plata region (RPtide model). The models were calibrated using water level series and salinity recorded at the area. The obtained hydrodynamic results show that the main dynamic of the area is well represented. In order to reduce computational times an empirical approach was used to determine which routines represent the main bottlenecks regarding execution time. After some code modifications, important acceleration factor values were obtained: 1.7 for RPtide and 3.0 for AStide case.

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