The impact of various types of open boundary conditions in numerical simulation of the Black Sea coastal circulation

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Abstract. An important problem is to obtain a short-term forecast in the Black Sea coastal zone with a high resolution. It is solved on the basis of numerical modeling of ocean circulation. Carrying out simulations that allow reproducing the meso- and submesoscale processes in a reasonable machine time requires a considerable computational power. One of the common ways to solve this problem is to create a regional configuration (a nested domain). This work is performed to study the influence of methods of specifying open boundary conditions. To conduct such a study, a regional configuration corresponding to the southern coast of Crimea with a resolution of 1.5 km is developed. Four short-term numerical experiments are carried out to investigate the influence of various types of open boundary conditions on the simulation results. The results of the simulations have shown that for a correct reproduction of the hydrophysical parameters, barotropic velocities at the open border should not be taken into account. At the open boundary, in the fields of temperature and salinity, there is no numerical noise when using a flow relaxation scheme. The sea level is reproduced correctly when using a Flather-type scheme.

1. Introduction
Since 2012, Marine Forecasting Center has been established at the Marine Hydrophysical Institute of RAS (MHI). It is still operating, allowing one to obtain information on the general circulation in the Black Sea in a real-time mode with quite good resolution (about 5 km). This system rather accurately describes the main features of the general circulation and the vertical structure of the basin: the Rim Current, its meandering, the location of mesoscale eddies, the depth of the cold intermediate layer (CIL), etc. To increase the quality of marine forecasts, reproduction of the large-scale processes is not sufficient. One should increase the resolution of the forecasting model to meso- and submesoscales. Processes of such scales are usually observed in the coastal and shelf areas. In these areas, a spatial resolution of ~ 5 km is not sufficient to adequately reproduce dynamic structures. In the coastal and shelf areas, both quasi-persistent and moving eddies of various scales and intensities are constantly observed. Therefore, reconstruction of the dynamics in the coastal areas should be carried out with a finer spatial resolution. Carrying out high-resolution simulations of the entire basin for an adequate machine time requires large computing capabilities. One of the solutions is modeling with an approach of nested grids. This method allows one to perform model runs of the restricted area of investigated domain using a fairly small grid step.

Due to small scales of the coastal processes, simulation results need to be validated against different types of observations obtained from a sub-satellite polygon. For the Black Sea, such studies are possible using data from the Black Sea Branch of MHI.
Considering the Black Sea basin, such studies are carried out at MHI by means of a numerical circulation model developed in [1]. Most of them are devoted to the reconstruction of currents of the northwestern shelf of the Black Sea [2]. This area, as the shallowest part of the basin, is of great interest for study. Another part of the studies is devoted to the reproduction of thermohaline fields and circulation in the coastal area of Crimea [3]. Upwelling phenomena are observed in this region. The vicinity of the Rim Current to the coast affects the generation of a large number of mesoscale and submesoscale eddies. Also, less salty and warmer waters of the Azov Sea flowing through the Kerch Strait spread along this coast. The results of numerical simulations in the described areas are verified with in-situ data of ARGO buoys, field data of Black Sea polygons, and during cruises of the R/V Professor Vodyanitsky.

When creating a nested domain or a regional configuration, the main impact on the internal region is carried out by setting open boundary conditions. A problem arises of setting open boundary conditions in the computational domain. A wide variety of methods for setting open boundary conditions is associated with the features that arise during their implementation [4], [5], [6]. The circuits described in [4] accumulate energy and cause a recirculation problem along the open boundary. To correctly reproduce the tidal impact in [5], a modification of the tidal scheme for the ROMS model is proposed. Some features of the implementation of the Flather scheme for barotropic variables and the scheme proposed by Orlanski for baroclinic velocities are given in [6].

Within the framework of the RSF project, MHI plans to create a nowcast/forecast system of the entire oceans [7]. To obtain a forecast in the Black Sea basin, the NEMO (Nucleus for European Modeling of the Ocean) [8] model will be used. It is well parallelized and well established in European forecast centers. Therefore, it is used in this work, whose purpose is to reproduce thermohaline fields in the coastal zone off the southern coast of Crimea. The main goal of the work is to study the influence of methods for setting open boundary conditions on the results of numerical modeling.

In this paper, the first part describes the model used to achieve the goals and the boundary conditions used in the calculations. The second part is devoted to a description of the configurations used in the calculations. The third part is devoted to an analysis of the influence of boundary conditions and a comparison of the results with the results of the basin configuration.

2. Methods and materials

2.1. Brief description of the OGCM and open boundary conditions

This study was carried out mainly using the NEMO (Nucleus for European Modeling of the Ocean) modeling framework [8]. The ocean component of NEMO (OPA) is based on primitive equations. Choosing an orthogonal set of unit vectors $\mathbf{i}, \mathbf{j}, \mathbf{k}$ ($\mathbf{k}$ is the local upward vector, and $\mathbf{i}, \mathbf{j}$ are two vectors orthogonal to $\mathbf{k}$), the equations are as follows:

\[
\frac{\partial U_h}{\partial t} = - \left[ (\nabla \times U) \times U + \frac{1}{2} \nabla (U^2) \right]_h - \mathbf{k} \times U_h - \frac{1}{\rho_0} \nabla_h p + D_U + F_U, \quad (1)
\]

\[
\frac{\partial p}{\partial z} = -\rho g, \quad (2)
\]

\[
\nabla \cdot U = 0, \quad (3)
\]

\[
\frac{\partial T}{\partial t} = -\nabla (TU) + D_T, \quad (4)
\]
\[
\frac{\partial s}{\partial t} = -\nabla (SU) + D^s, \quad (5)
\]

\[\rho = \rho(T, S, p), \quad (6)\]

\[w = \frac{\partial \eta}{\partial t} + U_{h|z=\eta} \cdot \nabla_h(h) + P + R - E, \quad (7)\]

where \(U\) is the current velocity vector; \(U_h\) is the current velocity in the \((i,j)\) - plane; 
\(f = 2\Omega k\) is the Coriolis acceleration; 
\(\Omega\) is the Earth’s angular velocity vector, 
\(\eta\) is the sea surface height, 
\(P\) is the precipitation, 
\(R\) is the river runoff, 
\(E\) is the evaporation; 
\(F^U\) are the surface forcing terms; 
\(D^U, D^T, D^S\) are the parameterizations of small-scale physics for the momentum, temperature, and salinity.

The equation of state (6) is the UNESCO formula [9]. The time splitting scheme is used for the calculation of the sea-surface height [10].

The system of equations is discretized using Arakawa’s “C” grid [11]. We use the vector invariant form of the momentum equation (1) with the energy and enstrophy conservation scheme [12]. The TVD scheme [13] is used for the discretization of the nonlinear terms in the transport–diffusion equations (4) and (5). The vertical mixing is described using a \(k-e\) turbulent closure model [14].

In NEMO, for each open boundary set a boundary condition has to be chosen for the sea-surface height, barotropic and baroclinic velocities, temperature, and salinity. We can choose a scheme for each variable. In this research, three of them are considered.

The Flow Relaxation Scheme (FRS) applies a simple relaxation of the model fields to externally-specified values over a zone next to the edge of the model domain [8],[15]. Given a model prognostic variable \(\Phi\),

\[\Phi(d) = \alpha(d)\Phi_e(d) + (1 - \alpha(d))\Phi_m(d); d=1,N,\]

where \(\Phi_e\) is the specified external field; 
\(\Phi_m\) is a model solution; 
\(d\) is the discrete distance from the boundary of the computational domain, and \(\alpha\) is a parameter that varies from 1 at \(d = 1\) to a small value at \(d = N\). The function \(\alpha(d)\) is specified as a \(tanh\) function:

\[\alpha(d) = 1 - \tanh\left(\frac{d - 1}{2}\right); d=1,N\]

Thus, the model solution is completely prescribed by the external conditions at the edge of the model domain and is relaxed towards the external conditions over the rest of the FRS zone. The application of a relaxation zone helps to prevent spurious reflection of outgoing signals from the model boundary. The parameter \(d\) usually ranges from 8 to 10.

The Flather scheme is a radiation condition on the normal, depth-mean transport across the open boundary [8,16]. It takes the form:

\[U = U_e + \frac{c}{h}(\eta - \eta_e),\]
where $U$ is the depth-mean velocity normal to the boundary and $\eta$ is the sea surface height, both from the model. The subscript $e$ indicates the same fields from external sources. The speed of external gravity waves is given by $c = \sqrt{gh}$, and $h$ is the depth of the water column. The depth-mean normal velocity along the edge of the model domain is set equal to the external depth-mean normal velocity, plus a correction term that allows gravity waves generated internally to exit the model boundary.

When using Dirichlet boundary conditions the values at the boundary of the region are equal to the values from the external (basin) configuration.

2.2. Model setup and numerical experiments

A regional configuration with a spatial resolution of $\approx 4.6$ km ($\frac{1}{24}^\circ$) was developed recently as the starting point for the new version of the Black Sea Marine Forecasting Center (BS MFC). However, the model domain covers cascading basins of the Azov, Black, and Marmara Seas (Figure 1). It can be considered as an extension of a configuration of the Black and Azov Seas proposed in [17]. The NEMO cascading configuration is being continuously adapted to the operational mode and validated against observations showing rather adequate results of the Black Sea general circulation and vertical structure, exchange through the Bosporus and Kerch Straits, the long-term salinity tendency in the Azov Sea [18].

Bearing in mind the location of the experimental polygon of the Black Sea Branch of MHI RAS, we choose an area covering the south-eastern coast of Crimea (Figure 1). As the starting point, the factor of 3 was used to produce the nested domain inferring the grid cell size is $\approx 1.5$ km. The bottom topography for the parent and child domains was prepared using an EMODnet bathymetry set [19] (Figure 1). The same setup of z-levels for the domains was used expecting further simulations using the nested grids technique.

The surface boundary conditions for the numerical experiments are based on the ERA5 product provided by the European Center for Medium-Range Weather Forecasts (ECMWF) [20]. The product has a spatial resolution of $0.25^\circ$ resolving the atmosphere mesoscale processes, and can be fairly satisfactory for the proposed study. Heat, mass, and momentum fluxes on the surface are obtained using a CORE bulk-formula [21].

The bilaplacian formulation is used for the representation of the lateral mixing ($D^U$, $D^T$, and $D^S$ in equations (1), (4) and (5). The long-term simulations of the general circulation in the cascading basins were made using values of $-5 \times 10^9$ m$^4$/s and $-4 \times 10^8$ m$^4$/s for the lateral turbulent viscosity and diffusion. Based on the results of preliminary simulations using a nested domain configuration, their values were chosen as large as $-5 \times 10^8$ m$^4$/s and $-5 \times 10^7$ m$^4$/s, respectively.

The free-slip boundary condition is used for the solid boundaries with a zero flux across the boundaries. On the bottom we use quadratic friction. No heat and salt flux condition is set for the temperature and salinity.

A preliminary free-run simulation for 1/1/2008 – 12/31/2008 was carried out using a configuration of cascading basins (basin). Conditions for temperature, salinity, baroclinic and barotropic velocities and sea-surface height prescribed on the liquid open boundaries for the nested domain configuration were obtained from respective results of a preliminary basin model run. After that, four model runs were performed using different combinations for prescribing open boundary conditions (Table 1). All experiments were carried out for the period of a month. The results of the experiments were compared with each other and with those obtained from the basin simulation.
Figure 1. Geographical location and bathymetry in the area under study: nested domain (dark-grey lines) within the domain of cascade configuration.

The Flather radiation scheme is prescribed for sea-surface height for all experiments. In the first experiment, the FRS was used for baroclinic velocities, and temperature and salinity. In the second experiment, the Dirichlet conditions were used for temperature and salinity, and baroclinic velocities were prescribed by the FRS (Table 1).

Table 1. Model runs and types of used open boundary conditions.

| Open boundary conditions | Sea-surface height | Temperature and salinity | Baroclinic velocity | Barotropic velocity |
|--------------------------|--------------------|--------------------------|---------------------|---------------------|
| Exp. 1                   | Flather            | FRS                      | FRS                 | none                |
| Exp. 2                   | Flather            | Dirichlet                | FRS                 | none                |
| Exp. 3                   | Flather            | Dirichlet                | none                | Flather             |
| Exp. 4                   | Flather            | FRS                      | none                | Flather             |

3. Results
Analyzing the spatial structure of simulated temperature and salinity, one can note their similarity. One can see that the sea water temperature on the first model level from exp. 1 and exp. 2 are rather close to the results obtained using the basin configuration. We can observe numerical noise at the lateral boundary in exp. 2, which is similar to two-step waves. They could appear due to the reflected wave. In the first experiment this is not observed, because a flow relaxation scheme was used for temperature and salinity, which prevents their appearance. The vertical temperature distribution in
these experiments is also close to the basin one. In experiment 2, at an open boundary numerical noise is observed to a depth of 100 m.

Figure 2. Sea water temperature (°C) on the first z-level for January 26, 2008.

The temperature and salinity fields in this simulation have different structures from the fields obtained in the basin configuration and in the first experiment (Figure 2).

The last, fourth experiment was carried out with the schemes used in the second experiment (sea-surface height - Flather scheme, barotropic velocities - flow relaxation scheme, temperature and salinity - Dirichlet type).

The results obtained in the last two experiments in the fields of temperature and salinity (Figure 2) have significant differences in the results of the basin configuration. The average temperature for the regional domain is close to experiments 1, 2, and 4. In the third experiment starting from January 8, the average temperature increases by 0.2 °C. Cyclone formation is observed in the center of the computational domain, which prevents the spread of warmer water from the Sea of Azov along the coast of Feodosia (Figure 2).

The formation of cyclone eddies can be more clearly observed in the field of flow velocities and in changes in the sea-surface height (Figure 3). The diameter of the cyclone is about 100 km. The reproducible cyclone exerts its influence on all levels. There is a significant decrease in the sea level in the center of the cyclone. In the first two experiments, the average sea-surface height is qualitatively close to each other and to the sea-surface height of the basin configuration.

The effect of using barotropic velocities in experiments 3 and 4 can be estimated by analyzing the average kinetic energy over the domain (Figure 4). The cyclone formation was directly reflected in the kinetic energy values. For the latest simulations it increased compared with the basin and experiments 1 and 2 by 10 times.
Since the last two simulations qualitatively poorly reproduce the thermodynamic parameters, it should be noted that barotropic velocities at the open lateral boundary should not be taken into account.

Analyzing the first part of the experiments, the following can be noted. In the first two simulations, the temperature and salinity fields are reproduced qualitatively and quantitatively close to the data obtained in the global configuration. In the first experiment, a flow relaxation scheme was used for these fields; numerical noise does not occur at the open lateral boundary, because this scheme prevents the appearance of waves reflected from the boundary. The use of barotropic velocities (experiments 3 and 4) leads to the appearance of a cyclone, which is not in the basin configuration. Its formation prevents the spreading of warm waters along the coast. It should be noted that the method of setting boundary conditions in the first experiment makes it possible to most faithfully reproduce the hydrophysical parameters being studied.
Conclusions
In the present study, a numerical simulation of physical parameters in the coastal area near the southeastern part of the Crimean Peninsula was performed. A nested grid configuration was developed with a spatial resolution of 1.5 km. Four short-term experiments were carried out with various types of open boundary conditions. In the fields of temperature and salinity at the open boundary there is no numerical noise when using the flow relaxation scheme. This scheme reduces or prevents the reflection of waves from the border. The sea-surface height is reproduced correctly by the Flather scheme. Analysis of the spatial structure of the simulated parameters has shown that for a correct reproduction of the hydrophysical parameters the barotropic velocities at the open boundary should not be taken into account. From this we conclude that the schemes selected in the first calculation most faithfully reproduce the hydrophysical parameters.

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