CHALLENGES FOR COUPLED MODELING OF INTER-BASIN EXCHANGE APPLIED TO TURKISH STRAIT SYSTEM

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1. Introduction

Many years after the first development by Kirk Bryan and his colleagues at GFDL (Geophysical Fluid Dynamic Laboratory) in the late 60s, ocean modelling today is still a very demanding research area utilizing modern science and technology. Despite great technological advances in high-performance computing and earth observation systems, the current understanding of the oceans fails to fully recognize complex multiple scale interactions characterizing these regions. Computationally demanding state-of-art modelling systems in use today either represent a limited spectrum appropriate for the particular geometry and grid, or parameterize corresponding processes. The development of fully coupled multi-component earth system models (ESMs) is a solid example of the promising new era in model development aiming to construct more complete, complex and robust modelling systems able to represent interactions among individual components of the often inhomogeneous and delicately coupled earth systems. It is clear that the next-generation ocean modelling systems will require new computational methods and advanced modelling to account for complex processes and data assimilated from new observation systems. In addition to the limited capability of current ocean models to resolve all too important smaller scales, the ocean is still vastly under-sampled to validate model results and produce better short-term forecasts. Models of basins interconnected by straits have to resolve small scale processes of hydraulic controls, turbulence and mixing in deep basins, straits, fjords etc., and have to consider their direct influences on the neighboring domains of the coupled basins. Likewise, mass budgets of coupled basins and their nonlinear free surface variations influence strait response, in return. Narrow straits such as the Bosphorus, Dardanelles, Messina and Gibraltar Straits provide ample evidence for all the complexity that arises as a result of coupling between straits and the adjacent ocean domains.

The multi-scale nature of systems of multiple basins interconnected through straits, coastal systems with a mosaic of fjords, estuaries, continental shelf and canyon geometries, regions of fresh-water influence or upwelling systems with inherently coupled elements make them individually challenging to study and understand, and even more so when such systems are coupled with each other. The short-term forecasting of these complex systems being already problematic, their multi-decadal and climate predictability yet needs greater care to preserve the capability to resolve the all too important smaller scales. In the end, the demands for accurate representation of physics quickly become counterweighed by computational demands, only to be partially relieved by innovation. Amongst such coastal systems, sea straits providing communication between sea basins have special ranking in complexity. Models of basins interconnected by straits have to resolve exchange flows influenced by hydraulic controls, turbulence, interfacial mixing, free surface variations and internal waves and possible tidal effects at the strait, as well as linked processes in the adjacent seas such as the full nonlinear variations of the free surface, realistic lateral and surface water and mass fluxes, intrusions of surface jets and bottom plumes issued from straits, continental shelf and internal mixing processes, surface and internal sloshing and the response of coupled systems to extreme weather conditions/events. Narrow straits such as the Bosphorus, Dardanelles, Messina and Gibraltar Straits provide ample evidence for all the complexity that could be envisioned, with also a series of closely connected actions in the adjacent seas.

2. Challenges in modelling of interconnected basins

The multi-scale ocean modelling of interconnected basins mainly involves coupling of hydrostatic, non-hydrostatic, turbulent and sea surface processes, further influenced by air-sea interaction, wind-wave dissipation and tidal effects (Lermusiaux *et al.* 2013). The diverse multi-component nature of the problem makes it challenging to study nonlinear interactions and feedback mechanisms among system components. The combined effects of processes at various temporal and spatial scales often presents a setback to investigate the dynamic response of the entire system as a whole, preventing a total understanding of the system. To that end, ocean models developed for interconnected basins must target to resolve the multi-scale dynamics of the ocean environment, from small scale turbulence in straits or passages to large scale circulation and gyres/eddies in the adjacent sea/s or semi-closed water bodies. Despite recent developments in ocean modelling in terms of dynamics, physical parameterizations and the numerical techniques (spatial discretization techniques, high-order schemes, adaptive unstructured meshing, nesting, grid generation and data assimilation), the multi-scale ocean modelling of interconnected basins coupled with straits, fjords and steep topographic features is still a very active and demanding research area that requires innovative state-of-art modelling tools to allow the entire system to be simulated, preferably based upon an easy to use, portable, efficient modelling framework. Modern developments in numerical ocean modeling and the increasing availability of computing resources have led to increasingly sophisticated models decreasing the number of simplifying approximations needed in the past and the need to couple non-hydrostatic and hydrostatic models to resolve multi-scale processes demands challenging new and full interpretations of the Navier-Stokes equations (Blayo and Rousseau, 2015).

One of the techniques to overcome difficulties in resolving details of processes in complicated ocean domains has been to devise methods allowing variable resolution where it is most needed inside the model domain. Over the last decade, the surge of interest in unstructured mesh methods resolving complex domains (i.e. straits, overflows and the continental break) have led to improved new ocean models such as ADCIRC (Westering *et al.* 1992), FVCOM (Chen *et al.* 2003) and FESOM (Danilov et al, 2004; Wang *et al.* 2008) allowing to refine the computational grid in desired sub-regions (Danilov, 2013). Often, spurious modes maintained in unstructured-mesh models have made them computationally more demanding compared to structured-mesh models (Danilov, 2013). Additionally, the multi-resolution functionality provided by the unstructured meshes are 2 to 4 times more expensive per degree of freedom than the structured-mesh models (Danilov, 2013). The difficulties in implementation of numerical methods (i.e. data assimilation systems and open boundary conditions) still prevent or limit the usage of the unstructured mesh ocean models to represent complex regional systems. The design of data assimilation systems in adaptive or multi-resolution mesh is more difficult than building a forward model, while using an adaptive mesh for the adjoint calculation has its own numerical requirements and difficulties (Weller *et al.* 2010). The implementation of conservation of the mass and energy in adaptive type meshes is also crucial problem because spurious waves can be generated in the adaptation phase of the mesh that eventually dominate the solution.

On the other hand, the well-known finite-difference methods in ocean modelling are based on structured meshes. When compared with unstructured mesh models, these models have poor representation of the coastlines especially for coarse resolution cases and it is often difficult to enhance the resolution of the underlying grid in a particular region even when curvilinear coordinates and nesting strategies are employed. These problems also prevent realistic use of structured grid ocean models in applications involving interconnected basins, where excessive local refinement of the model grid to fine-scale components (i.e. straits) is needed. To overcome difficulties in designing structured grids in complicated domains, the composite or multi grid approach was developed and applied in the 90s. For example, Eby and Holloway (1994) investigated the grid transformation approach to couple separate model domains of the Artic region and the global ocean. In their design, the information along common boundaries were passed between the two model components in each iteration of the solver. Similarly, Dietrich *et al.* (2008) designed a multiple-grid ocean model to study the effects of the Mediterranean Overflow Water (MOW) in the North Atlantic Ocean, where a seamless integration between grids of different spatial resolution were achieved by using the method of upwind boundary fluxes developed by Dietrich *et al.* (2004). A similar composite grid approach has been used to study residence time in a partially mixed estuary (Warner *et al.* 2010), making sure that the numerical solution in each grid would not be different from the solution in a single grid including the entire domain. To simplify the coupling between multiple grids, the overlap regions are often forced to be coincident (all grid properties are identical in overlapping grid cells). In this case the domains could actually be merged into a single grid alleviating the need for composite grids of different resolution, such as needed in the case of interconnected basins. Coupling of models with different dynamical cores (e.g. hydrostatic and non-hydrostatic) and physical parameterizations often required in multi-scale ocean modelling (e.g. interconnected basins) is not possible in this approach.

In addition to the possible use of a single monolithic grid to represent various scales, the nesting approach is often used in ocean modeling to bridge across coarse and fine scales. For time-dependent problems, adaptive mesh refinement (AMR) allows dynamically adjusted resolution, such as in the AGRIF (Adaptive Grid Refinement in Fortran; Debreu *et al.* 2008) package, discretized on a structured grid. Successful application of the nesting approach by Sannino *et al.* (2009) demonstrated the influence of the Strait of Gibraltar on the water column stratification and convection in Mediterranean Sea, allowing better representation of hydraulic control in the strait for improved estimates of volume transport and Mediterranean Outflow Water (MOW; Dietrich *et al.* 2008). Although the nesting approach is quite common in ocean modeling, the representation of interconnected basins like the TSS still poses a challenging problem. Moreover, the two-way data exchange among the nested models is also problematic and might create mass conservation problems due to the interpolation, numerical errors and spurious mixing along the boundaries.

In essence, the behavior is reflected in the definition of a “system”- a set of interacting or interdependent components forming a complex whole. The Turkish Strait System (TSS) is a perfect example of the complex ocean modelling problem that can be posed for such systems. It is a unique environment to study exchange flows, hydraulic controls, turbulence, internal waves, subject to externally imposed net water flux variability, extreme weather events, storm surges, internal sloshing and tidal effects. The combined effects of these processes are essential to determine the overall system response, which actually is a demanding problem of coupled ocean modelling.

3. Challenges in modelling of Turkish Strait System

The oceanographic conditions of the TSS has been extensively well investigated in the last thirty years. The variability of currents and other physical properties are well established, although the much needed coastal observatories are lacking. The basic dynamics creating the two-way exchange flows of the TSS are the density and pressure differences between the Black and the Aegean Seas, first revealed by Marsili (1681) studying the Bosphorus three centuries ago (Defant, 1961; Soffientino and Pilson, 2005; Pinardi, 2009; Pinardi *et al.* 2016). The TSS is very sensitive to climatic changes, and potentially can induce such changes in the adjacent basins (Özsoy, 1999). Acting as the limiting element of the TSS, the Bosphorus Strait controls the exchange of mass and materials between the Black and the Mediterranean Seas (Ünlüata *et al.* 1990; Özsoy *et al.* 1995; Polat and Tuğrul, 1995), thereby influencing the stratification, water and mass budgets (Özsoy *et al.* 1993; Özsoy and Ünlüata, 1997, 1998; Delfanti *et al.* 2014; Falina *et al.* 2016; Jordà *et al.* 2016). The mass budget dictates the upper layer flux to be about two times larger than that of the lower layer, yielding a net flux of about 300 km^3/yr from the Black Sea to the Sea of Marmara (Latif *et al.* 1991; Ünlüata *et al.* 1990). Geometrical features of the Bosphorus (Oğuz *et al.* 1990; Özsoy *et al.* 1998) imply 'maximal exchange', as proposed by Farmer and Armi (1986) influenced by local topographic features. The exchange flows respond dynamically to time-dependent hydro-meteorological forcing in the adjacent basins (Özsoy *et al.* 1995a, 1996, 1998; Gregg and Özsoy, 1999). Observations suggest increased entrainment past the hydraulic controls at the southern contraction and the northern sill in the Black Sea (Gregg *et al.* 1999, 2002; Özsoy *et al.* 2002).

The Sea of Marmara possesses a two-layer stratification and associated flow system, in which an approximately 25 m layer of relatively less saline (salinity ~25) water mass of the Black Sea origin is separated from the rest of the water body by a sharp permanent pycnocline. The two-layer structure is preserved even in the winter season when abrupt cooling of surface waters increases the density of the upper layer by about 1-2 kg/m^3. The corresponding flow system in the sea reveals a stronger circulation in the upper layer with a preferential direction towards the Aegean Sea. The upper layer circulation inferred from the existing hydrographic data (Beşiktepe *et al.* 1995) suggests the presence of a large anti-cyclonic loop of the surface flow upon issuing from the Bosphorus. As this larger scale flow system is generally controlled by seasonal wind forcing, evolution of the surface buoyant jet of the Bosphorus surface outflow by horizontal and vertical entrainment processes near the Bosphorus-Marmara junction region adds further complexity to the regional circulation. The currents in the lower layer is much weaker, and the time scale of their transit across the sea towards the Bosphorus is approximately an order of magnitude longer than that of the surface layer. The exchange flows respond dynamically to forcing on time scales from several days to years by wind setup, water budgets and atmospheric pressure differences. Three dimensional hydrodynamic models have been used to investigate exchange flows under ideal conditions of the Bosphorus Strait and need to be further developed for application to the Bosphorus and Dardanelles Straits. The conditions in the Marmara Sea connected to the outlying seas by the Bosphorus and Dardanelles Straits are also relatively well known, although its complex nature with a wide shelf and deep basins, and severe winter weather conditions often create complex currents and meteorology that justifies further careful consideration of risks concerning navigation and the environment.

The strategy of recent studies aiming to understand the TSS necessarily has been a divide-and-conquer approach to decompose/isolate individual components and very few modelling studies have attempted to study the integral behavior of TSS considering contrasting properties and nonlinear interactions of its sub-components. In this case, the existing modelling studies have passed through a series of successive developments, starting from two and three dimensional models with idealized geometry and extending to realistic three-dimensional ocean models applied to individual elements of the system.

Idealized two-layer, one-dimensional or two-dimensional models solving horizontally or vertically integrated hydrodynamic equations have been developed for the Dardanelles Strait (Oğuz and Sur, 1989; Staschuk and Hutter, 2001) as well as the Bosphorus Strait (Oğuz *et al.* 1990; Ilıcak *et al.* 2009). Three-dimensional models solving full set of primitive equations have later been developed for the Dardanelles Strait (Kanarska and Maderich, 2008) and for the Bosphorus Strait (Sözer and Özsoy, 2002a and 2002b; Oğuz, 2005; Sözer, 2013; Sözer and Özsoy, 2016). In addition to these models developed for straits, some earlier studies have aimed to treat Marmara Sea as an isolated marine basin, with the addition of artificial inflow and outflow sources at the Bosphorus and Dardanelles Straits, thereby decoupling the dynamics of the straits from the basin (Demyshev and Dovgaya, 2007; Demyshev, 2012 and Chiggiato *et al.* 2011). The main problem of all these approaches rest in ignoring the interactions among various components, by imposing inappropriate boundary and initial conditions to subsystems of the TSS. Although models representing the individual components of the entire system are definitely valuable tools for analyzing the hydrodynamic behavior of those components, recent studies using integrated modelling of the TSS by Gürses *et al.* (2016) and Sannino *et al.* (2016) showed that the TSS hydrodynamics cannot be adequately understood or even resolved, unless the details of the very substantial dynamics of the straits are included in full detail in the essentially coupled system. The nonlinear, strongly stratified hydrodynamics of the flow through the narrow straits has made the modelling of TSS a grand challenge because of the need to resolve the straits in fine detail, which typically are not elaborated in modelling applications concerning open oceans and coastal regions (Sannino *et al.* 2016).

Specifically, in the case of the Turkish Straits System (TSS), surface water jets and bottom plumes generated in the Black, Marmara and Aegean Seas and the intrusion of water masses into the adjacent seas have to be accounted for, essential for driving the Marmara Sea circulation and with particular effects on the double diffusive instability regime of the Black Sea. Representing these fine scale features, at the same time insisting on conservation of mass and energy among the components of interconnected system are essential for models. There is an obvious need for current state-of-art modelling tools to be developed using model coupling frameworks/libraries at the required level of sophistication (in terms of both physics and computational methods) to facilitate the construction of innovative modelling systems and their applications.

4. Towards multi-instance and multi-component ocean models for interconnected basins

As briefly mentioned in the previous sections, the development of methods for systematic coupling of multiple marine basins and straits has never been formally attempted in the past. The intended novel design is based on coupling multiple realizations of high resolution ocean model components, surpassing the earlier concepts of trying to fit the entire system in a single model application, destined to fail in the accurate representation of temporal and spatial characteristics of each sub-system. The multi-instance ocean modeling (MIOM) system aims to create specialized coupling tools linking separate components of the system irrespective of size and structure, thus enabling to study multi-scale processes in the interconnected system. The higher-level modelling system basically acts to orchestrate simultaneous operation of individual marine components by allowing two-way interactions among them and also with the active atmosphere model. The TSS is a perfect example to test and develop such modeling system, given its complex internal dynamics coupled with the near-field and remote effects of two large basins.

The design of such a complex modelling system (MIOM) presents a set of difficulties in employing independently developed model components for different parts of the domain. Each model component could have different horizontal and vertical grid structure and spatial resolution. In this case, specialized tools such as model coupling libraries and frameworks are used to couple different model components. The Earth System Modeling Framework (ESMF; Hill et. al., 2004a and 2004b; Collins et. al., 2005), Model Coupling Toolkit (MCT, Jacob *et al.* 2005, Larson et. al., 2005), Model Coupling Environmental Library (MCEL, Bettencourt, 2002), OASIS (Redler *et al.* 2010, Valcke, 2013) and C-Coupler (Liu *et al.* 2014) can be given as examples of methods simplifying the regular tasks in creating a coupled modelling system. To tackle the problem, the MIOM will use driver based model coupling approach based on the ESMF coupling framework. The ESMF framework is selected because of its unique online three-dimensional re-gridding capability, which allows the driver to readily perform interpolation over the exchanged fields (i.e. temperature, salinity, heat and momentum fluxes) using the National Unified Operational Prediction Capability (NUOPC) layer. The NUOPC layer basically simplifies common tasks of model coupling, component synchronization and run sequence (i.e. implicit, semi-implicit and explicit type of coupling) by providing an additional wrapper layer between coupled model components and the ESMF framework (Figure 1).

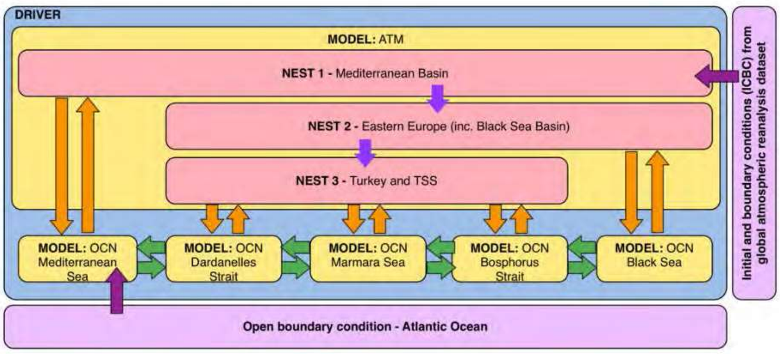

Figure 1 Design of multi-instance ocean model (MIOM) and coupling with active atmosphere component for TSS.

In the proposed ocean modelling system of MIOM, individual ocean model components exchange information (i.e. water fluxes, tracers) along their overlapped regions that are called buffer zones or dynamic interfaces. In this case, the seamless integration of model components requires mapping of exchange fields (i.e. temperature, salt, velocity components) among different instances of the modelling system using conservative methods of interpolation to prevent addition of artificial heat, momentum and mass fluxes by exchanging fields. A possible disadvantage of this method is that the model instances do not constrain the interior of the counterpart model instance directly, and there is nothing to prevent unrealistic drift of the model instances and/or sharp gradients of fluxes between the model components. A method to solve this problem is to apply flux balancing algorithm such as a revised version of the smoothed semi-prognostic (SSP; Greatbatch *et al.* 2004) method used in two-way nesting of ocean models (Sheng *et al.* 2005) to balance fluxes between adjacent model instances.

As it is mentioned before, the developed models of TSS uses relatively low-resolution offline atmospheric forcing to drive the individual components of the TSS model and it neglects the two-way interaction and feedback mechanisms in the air-sea interface that might have a vital importance in the response of the overall system to the atmospheric conditions especially for the blocking problems in the straits and water mass exchanges through the straits by modifying evaporation from the Mediterranean and Black Seas surfaces. Additionally, the previous study of Turunçoğlu and Sannino (2016) showed that the coupled atmosphere-ocean model tends to modify the heat fluxes in the air-sea interface of the Mediterranean Sea by reducing the latent heat loss from the sea surface and the rate of change of latent heat flux might reach up to %10 especially in Eastern Mediterranean. The decrease of evaporation over the sea also affects the precipitation over the sea due to the reduction of moisture content of the lower atmosphere. It is clear that the nonlinear air-sea interaction should play an important role in the dynamics of the TSS system and mass transport through the straits. The coupling of MIOM system with a fully active atmosphere component is expected to reduce biases by improved representation of the air-sea interface. The coupling of MIOM system with an active atmospheric component will be the first attempt to design and test a novel modeling approach to integrate the different earth system model components to represent the entire TSS.

The earlier studies investigating the hydrodynamic behavior of the TSS have focused on individual components of the system either coupled with or in the absence of complicating atmospheric effects. The previous study of Chiggiato *et al.* (2011) only included the two Straits as open boundaries (inflow and outflow sections) and used atmospheric forcing at 7 km spatial resolution to simulate the mainly wind-driven circulation superposed on the basic flow imposed through the straits. It is clear that the horizontal resolution used by Chiggiato *et al.* (2011) is still insufficient to study the detailed response of the very narrow straits to atmospheric conditions. Due to the multi-scale nature of the region of interest, the horizontal resolution of required atmospheric forcing for modelling entire TSS and the bordering seas are not uniform. While the required horizontal resolution of atmospheric forcing for Marmara Sea is around 5-10 km (internal Rossby radius of deformation is estimated to be around 17 km by Chiggiato *et al.* 2011), higher resolution atmospheric forcing of 1-3 km is required to study water transport and circulation in very narrow straits. The various horizontal resolution requirements of the study lead the usage of nesting strategy to perform atmospheric simulations. Accompanying the nested domain configuration with desired horizontal resolution, a non-hydrostatic regional atmosphere model will provide high-resolution atmospheric forcing for the entire modeling system (MIOM). The use of a non-hydrostatic model allows to add additional inner-most nests over straits with enhanced horizontal resolution for better representation of local effects such as complex coastlines and steep topography.

The methodology developed will provide the much needed tools to examine seemingly hidden details in a functional prototype and open up new opportunities to understand the complex feedback mechanisms and interactions which are crucial in the development of forecasting capabilities. The approach also employs a development strategy that would allow addition of other components as needed in the future, using the same methodology: for instance hydrological models of river catchments can be added as land components supplying riverine and overland flow components, or biochemical model components representing marine ecosystems.

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