Ocean Modelling 92 (2015) 56–68

Contents lists available at ScienceDirect

Ocean Modelling

journal homepage: www.elsevier.com/locate/ocemod

Virtual Special Issue
Coastal ocean modelling

Advantages of vertically adaptive coordinates in numerical models of stratified shelf seas

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ARTICLE INFO

Article history:
Received 9 February 2015
Revised 10 May 2015
Accepted 28 May 2015
Available online 5 June 2015

Keywords:
Stratification
Adaptive coordinates
Numerical mixing
GETM
North Sea
Baltic Sea

ABSTRACT

Shelf seas such as the North Sea and the Baltic Sea are characterised by spatially and temporally varying stratification that is highly relevant for their physical dynamics and the evolution of their ecosystems. Stratification may vary from unstably stratified (e.g., due to convective surface cooling) to strongly stratified with density jumps of up to 10 kg/m^3 per m (e.g., in overflows into the Baltic Sea). Stratification has a direct impact on vertical turbulent transports (e.g., of nutrients) and influences the entrainment rate of ambient water into dense bottom currents which in turn determine the stratification of and oxygen supply to, e.g., the central Baltic Sea. Moreover, the suppression of the vertical diffusivity at the summer thermocline is one of the limiting factors for the vertical exchange of nutrients in the North Sea. Due to limitations of computational resources and since the locations of such density jumps (either by salinity or temperature) are predicted by the model simulation itself, predefined vertical coordinates cannot always reliably resolve these features. Thus, all shelf sea models with a predefined vertical coordinate distribution are inherently subject to under-resolution of the density structure.

To solve this problem, Burchard and Beckers (2004) and Hofmeister et al. (2010) developed the concept of vertically adaptive coordinates for ocean models, where zooming of vertical coordinates at locations of strong stratification (and shear) is imposed. This is achieved by solving a diffusion equation for the position of the coordinates (with the diffusivity being proportional to the stratification or shear frequencies). We will show for a coupled model system of the North Sea and the Baltic Sea (resolution ~ 1.8 km) how numerical mixing is substantially reduced and model results become significantly more realistic when vertically adaptive coordinates are applied. We additionally demonstrate that vertically adaptive coordinates perform well in simulating the two dynamically different regions North Sea and Baltic Sea with a single parameter set.

An analysis of the computational overhead of the adaptive coordinates indicates an increase of 5–8% in runtime. This is still less expensive than adding more sigma-layers to reduce spurious numerical mixing.

1. Introduction

In shelf seas processes at horizontal interfaces play a pivotal role for the marine ecosystems. Important interfaces are external interfaces such as the sea surface, and the sea bed and internal interfaces such as thermoclines, haloclines and lutoclines, but also thin layers of e.g. phytoplankton.

Near the air–sea interface, all fluxes between ocean and atmosphere directly depend on vertical gradients of properties in the upper few metres of the water column, see e.g. McGillis and Wanninkhof (2006) for fluxes of CO_2. Complex hydrodynamics including, wind–wave–current–turbulence dynamics occurring on vertical scales of a few metres, are substantially influencing air–sea fluxes and near-surface turbulent fluxes (Sullivan and McWilliams, 2010). A similar situation is present at the sea bed, where the turbulent bottom boundary layer mediates sediment-water fluxes of solutes or particulate matter into the water column (e.g., Holtappels et al., 2011). On the other hand, settling of suspended particulate matter (SPM) depends on the near bottom SPM concentration (Jones et al., 1996). In many shelf sea regions, the near-bed area is characterised by thin fluffy SPM layers with substantial oxygen depletion (see Howarth et al., 2002 and references therein). In one-dimensional coupled

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http://dx.doi.org/10.1016/j.ocemod.2015.05.008
1463-5003/

physical–biogeochemical models of the water column, it is generally no problem to obtain a sufficiently high resolution near the sea surface or the sea bed (Burchard et al., 2006).

However, substantial problems occur in three-dimensional models due to the slope of the seabed and the spatio-temporal variation of the sea surface elevation. Classical models with geopotential (z-level) vertical coordinates Griffies et al. (2001) are typically limited in their near-surface resolution by the range of the maximum surface height variation which may be in the order of a few metres. Such problems could be solved by introducing a so-called z^* coordinate where the layers thicknesses defined by the original z levels are compressed or expanded to account for temporal changes in water depth Adcroft and Campin (2004), therefore allowing for arbitrarily high near-surface resolution. However, a zooming of layers towards the sloping sea bed is not possible such that typical near-bed vertical resolutions of geopotential coordinate models are in the order of a few metres (Pohlmann, 2006). Furthermore, such models approximate the sloping seabed in a staircase-like manner, a feature that impedes undisturbed flow along the bottom. A work-around has been proposed by Beckmann and Döscher (1997) who directly connected all bottom boxes by means of a terrain-following bottom boundary layer model. Although allowing for down-slope transport of tracers, this method does not provide increased vertical resolution near the bed. This problem is partially solved by surface and bottom following σ coordinates (with $\sigma = (z - \eta)/(H + \eta)$, the undisturbed water depth H, the geopotential coordinate z and the sea surface elevation η). Since σ coordinates define layer thicknesses that vary proportionally to the spatio-temporal variations of the water depth, the near-bottom and near-surface resolutions are coarsened in deep water. This problem has been solved by introducing non-linear general vertical coordinates that may be constructed in a way that overall high resolution of boundary layers is obtained (Burchard and Petersen, 1997; Gerdes, 1993; Song et al., 1994). The vertical s coordinate is the vertical discretisation which is commonly used in modern shelf sea models such as in the Regional Ocean Modelling System (ROMS, Shchepetkin and McWilliams, 2005) and in the General Estuarine Transport Model (GETM, Burchard and Bolding, 2002; Hofmeister et al., 2010; Klingbeil and Burchard, 2013). Burchard and Petersen (1997) show that the well-known pressure gradient problem inherent for σ coordinate models Haney (1991) can be significantly reduced when s coordinates or hybrid coordinates combining σ and z coordinates Gerdes (1993) are used.

While s coordinates appear as a robust solution for resolving the surface and the bottom boundary layers, vertical gradients due to interfaces in the interior may not be sufficiently resolved. Simply increasing the number of vertical layers is usually not possible, since the computational effort would exceed practical limits. Isopycnal coordinates using density levels as coordinate levels had been introduced long ago to resolve the dynamics of pycnoclines in an efficient way (Bleck and Smith, 1990; Oberhuber, 1993). Due to limitations in resolving boundary layers and areas of neutral or unstable stratification, the isopycnal coordinate concept has been combined in a hybrid method with σ and z coordinates to ensure appropriate resolution where needed (see the ocean model HYCOM, Bleck, 2002).

An alternative and generalised approach of vertically adaptive coordinate has been proposed by Burchard and Beckers (2004). Exploiting the concept of general vertical coordinates (Kasahara, 1974), they solve a diffusion equation for the position of the vertical layers, where the diffusivity is proportional to stratification, shear, proximity to sea surface or sea bed and a background (back to σ) value. This method ensures increased vertical resolution at locations of increased shear or stratification. Later, Hofmeister et al. (2010) extended this one-dimensional coordinate optimisation method to three-dimensional models by adding Lagrangian and isopycnal tendencies, as well as lateral coordinate smoothing. They could show that the pressure gradient error was substantially reduced using this method. Additionally, numerical mixing could be reduced by minimising the grid-related vertical velocity. This is a consequence of the feature that the adaptive grid is following vertical oscillations due to internal waves or tides. Hofmeister et al. (2011) showed that a major salt water inflow event into the semi-enclosed Baltic Sea could be reproduced with much higher accuracy using vertically adaptive coordinates. Using the numerical mixing analysis by Burchard and Rennau (2008) they found that the contribution of numerical mixing to the total mixing (physical plus numerical) was reduced from 80 to 50%. In contrast to the simulated inflow using sigma coordinates, which did not reach the central Baltic Sea, the simulations with adaptive coordinates reproduced observations of the arrival of the saline plume.

The present paper intends to analyse the performance of vertically adaptive coordinates for a complex multi-decadal simulation of the coupled North Sea–Baltic Sea system (NSBS). This shelf sea system includes for the North Sea tidal dynamics with strong tidal ranges, tidal fronts, seasonal thermal stratification, internal tides, and large homogeneously mixed regions. In the Baltic Sea the model is challenged by dense bottom currents, distinct upwelling areas, boundary mixing, large quiescent stratified areas and partially very strong stratification. The quality of the model simulations is assessed using various types of long-term and high-resolution observations.

The outline of the paper is as follows: in Section 2 we give an overview of the used validation data. Moreover, we introduce the mixing analysis to distinguish and to quantify the effects of physical and numerical mixing. Section 3 deals with the description of the ocean model. It also presents the experimental design to study the differences between s coordinates (SC) and adaptive coordinates (AC). In Section 4 we present some validation results to prove that the model system with adaptive coordinates is able to reproduce the state of the North Sea/Baltic Sea for the period 1997–2012. We also compare our results with recent state estimates based on data assimilation. In Section 5 we present a thorough analysis of SC and AC based on a twin experiment. The comparison focuses on the differences between numerical and physical mixing and the resulting consequences. Finally, in Section 5, we summarise our findings.

2. Methods and data

2.1. Data

2.1.1. Stations

Sea level records have been obtained for nine sites around the North Sea and Baltic Sea (blue dots in Fig. 1). The sea level records have been converted into the same format and referenced in universal time +0 h. The mean of all time series, for both regions, has been removed to avoid biases due to different national reference heights, as we were only interested in the deviations from the mean and not in the absolute height. The data have been rigorously checked for common errors such as data spikes. Spurious records have been excluded. The observations have at least a temporal resolution of one hour. The observed time series have been separated into their three components: mean sea level, astronomical tide, and non-tidal residuals. This separation is performed by means of a separate tidal analysis for each calendar year, using the harmonic tidal analysis MATLAB toolbox T_TIDE of Pawlowicz et al. (2002). For the North Sea we compared the tidal and residual sea levels. For the Baltic Sea the gauge data were directly used for validation (without de-tiding), since tidal contribution are nearly absent.

The observational data for temperature and salinity show a much wider spread in temporal resolution than the gauge data. It ranges from hourly observations at permanent stations like Oysterground (OG) and Ems (in the North Sea), to nearly monthly CTD profiles as assessed by the HELCOM database for stations BY2, BY15 and US5B in the Baltic Sea (magenta dots in Fig. 1).