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A 3D, cross-scale, baroclinic model with implicit vertical transport for the Upper Chesapeake Bay and its tributaries

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ABSTRACT

We develop a new vertically implicit transport solver, based on two total variation diminishing (TVD) limiters in space and time, inside a 3D unstructured-grid model (SCHISM), and apply it to the Upper Chesapeake Bay (UCB), which has complex geometry and sharp pycnocline. We show that the model is able to accurately and efficiently capture the elevation, velocity, salinity and temperature in both the deep and shallow regions of UCB. Compared with all available CTD casts, the overall model skills have the mean absolute error of 1.08 PSU and 0.85 °C, and correlation coefficient of 0.97 and 0.99 for salinity and temperature respectively. More importantly, the new implicit solver better captures the density stratification, which has great implications on biogeochemistry in this estuarine system. The cross-scale capability of the model is demonstrated by extending the high-resolution grids into a tributary (Chester River) and its sub-tributary (Corsica River), with minimal impact on the model efficiency. The model is also able to capture complex 3D structures at the transition zone between the main bay and the tributary, including the three-layered circulation in Baltimore Harbor. As more and more attention is being paid to the productive shallows in the Chesapeake Bay and other estuaries, the model can serve as a very powerful management tool to understand the impact of both local and remote forcing functions.

1. Introduction

The Chesapeake Bay is the largest estuary in the USA, and provides essential habitats and ecosystem service for microbes, invertebrates, micro- and macro-fauna, and diverse fish species (Najjar et al., 2010). As a result, the Chesapeake Bay has stimulated a great deal of research interests, ranging from the understanding of the physical processes (Goodrich et al., 1987; Valle-Levinson et al., 2003; Scully et al., 2005), to eutrophication (Boesch et al., 2001; Cerco and Noel, 2004; Kemp et al., 2005), hypoxia (Officer et al., 1984; Bever et al., 2013; Du and Shen, 2015), and to the long-term trend of the above mentioned processes under climate change (Hagy et al., 2004; Najjar et al., 2010; Murphy et al., 2011; Hong and Shen, 2012). In recent years, increasing emphasis has been placed on the productive tributaries and shallow regions of the Chesapeake Bay, which have drawn particular interest from management (Cerco et al., 2013). In other estuarine and coastal systems beyond the Chesapeake Bay, there is also a universal need to investigate small-scale processes under large-scale remote forcing in a holistic manner (Brown and Ozretich, 2009; Möller et al., 2001; Gong and Shen, 2011).

Numerical models can serve as a powerful tool for understanding the past, projecting future changes and assisting decision-making. On account of the increasing emphasis on tributaries and shallow regions, cross-scale modelling capability is highly desirable in order to adequately address the intertwining processes on contrasting spatial and temporal scales. Previous numerical studies have been conducted with emphasis on various parts of the Chesapeake Bay. On the whole-bay scale, the Curvilinear-grid Hydrodynamics 3D model (CH3D) is currently serving as the regulatory model for the Environmental Protection Agency's Chesapeake Bay Program (Linker et al., 2002). CH3D is also included in the Chesapeake Bay model inter-comparison conducted by Irby et al. (2016). This inter-comparison demonstrated that all participating models performed nearly equally well in terms of reproducing stratification throughout the main stem of the Chesapeake Bay. However, the models were not compared in the shallower tributaries, largely

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because nearly all of the models utilized structured grids. The limited cross-scale capability of these models led to insufficient resolutions in the shallows and tributaries (Cerco et al., 2013). One- or two-way nesting approaches could partially mitigate these limitations, but would also likely produce transition issues at the boundaries between grids.

Unstructured-grid (UG) models are known to be ideal for cross-scale problems because of their superiority in resolving complex geometry/bathymetry, and flexibility in local refinements (Luettich et al., 1992; Casulli and Walters, 2000; Chen et al., 2003). We have made significant progress in developing state-of-the-art 3D baroclinic UG models and applying them to rivers, estuaries, shelf, and deep oceans (Zhang and Baptista, 2008; Zhang et al., 2015). As mentioned in Zhang et al. (2016), both accuracy and efficiency are important considerations in this endeavor. The large variation in element size and the fine resolution used in the vertical dimension have set a high bar for model stability. Models based on implicit time stepping, without the traditional mode splitting technique, are therefore particularly powerful for this type of applications, as large time steps can be used in conjunction with higher resolution. In the past, significant effort has been devoted to the calculation of the continuity and momentum equations with implicit methods (Casulli and Cattani, 1994), but relatively little attention has been paid to efficiently solve the 3D transport equation. Consequently, the latter now emerges as one of the most limiting factors for efficiency (Zhang et al., 2016). In particular, the higher-order transport solver is often inefficient, due to the stringent Courant number constraints, especially in the vertical dimension. This is because high resolution is required in the vertical dimension to capture the sharp gradients in the tracer concentrations. In an estuarine setting, a bottleneck frequently emerges at the locations of large bottom slopes or in shallow regions. This inefficiency issue is exacerbated as more tracers are advected. For example, a typical water quality simulation includes twenty or more tracers in addition to salinity and temperature.

Previously a novel technique has been proposed by Hodges (2014) that allows the use of different time steps at different locations (instead of enforcing the stability condition with a global time step for the entire grid). However, this formulation only applies to a particular type of transport equation, with the tracer mass (instead of concentration) as the dependent variable. Hybrid methods weighting explicit and implicit scheme based on local Courant numbers have been introduced by Gross et. al. (1998) and more recently by Shchepetkin (2015) to ocean models. An issue with these methods is that they do not ensure monotonicity, i.e. the tracer concentration may have over-/under-shoots ('negative mass' in some literature). This is tolerable in oceanic applications, where salinity is always much larger than zero and small undershoots won't create serious problems. In estuaries, however, zero concentration and sharp gradients in salinity and other tracers are ubiquitous, so a monotone advection scheme is critical. In the present work, we adopt the monotonicity-preserving scheme of Duraisamy and Baeder (2007), based on a direct second-order reconstruction in *both* space and time with two Total Variation Diminishing (TVD; (Harten and Lax, 1984)) limiters. We modify their temporal TVD limiter, and extend their 1D scheme to non-uniform grids with convergent/divergent vertical flows and account for surface boundary conditions. We demonstrate that the scheme is able to achieve high accuracy and at the same time high efficiency in numerical benchmarks and estuarine applications.

We have successfully incorporated the new solver into a 3D UG model, SCHISM (Semi-implicit Cross-scale Hydroscience Integrated System Model; Zhang et al., 2016) and applied it to the Upper Chesapeake Bay (UCB) and its tributaries. We chose the UCB rather than the entire Chesapeake Bay as a first step, mainly to reduce the uncertainties associated with the ocean boundary conditions and watershed inputs. This way, the performance of the newly introduced techniques (including the new transport solver described in this paper, as well as the highly flexible horizontal and vertical gridding systems in SCHISM) can be more objectively assessed. We obtain excellent results for elevation, velocity, salinity and temperature as well as stratification, in an efficient fashion. The model also successfully captures some distinctive circulation patterns between the main stem and the tributaries, namely the three-layered circulation near the mouth of Baltimore Harbor (Schubel and Pritchard, 1986; Chao et al., 1996). We also demonstrate the cross-scale capability of the model in Chester River, which is a small tributary of UCB and is an area of management interest due to its water quality issues (Kim and Cerco, 2003). With the success in the UCB, we are in the process of applying the same technique to a seamless shelf-bay-tributary model that covers the whole Bay and extends beyond the continental slope. This work will be presented in a subsequent paper. Our ultimate goal is to provide estuarine and coastal management with a holistic tool to easily understand the impact of both local and remote forcings.

In the following sections, we first provide the details of the new implicit transport solver and how it fits into SCHISM (Section 2), and then describe the set-up (Section 3) and validation (Section 4) of the UCB model. The sensitivity and cross-scale capability of the UCB model are discussed in Section 5, followed by conclusions in Section 6.

2. New transport solver

2.1. Formulation

The transport equation of a generic tracer can be written as:

$$\frac{\partial T}{\partial t} = -\nabla \cdot (\mathbf{u}T) + \frac{\partial}{\partial z}\left(\kappa \frac{\partial T}{\partial z}\right) + q, \quad (1)$$

where T represents the concentration of a generic tracer; κ is vertical eddy diffusivity (m^2 s^{-1}); q includes all source and sink terms; $\mathbf{u}$ is the three-dimensional velocity vector (u, v, w) (m s^{-1}). We have neglected horizontal diffusion in Eq. (1) for brevity, as its implementation is straightforward.

Previously, a 2nd-order finite-volume based explicit TVD (FV–TVD) scheme has been implemented in SCHISM (Zhang and Baptista, 2008; Zhang et al., 2015), which simultaneously ensures mass conservation and monotonicity via the maximum principle. However, FV-TVD often demands smaller time steps to ensure the stability for the whole domain. As a result, the majority of the elements operate with Courant numbers that are much lower than the maximum allowable Courant numbers locally, leading to inferior efficiency and some numerical diffusion. In order to relax this constraint, we introduce an implicit solver while maintaining the TVD property.

Vertical advection often imposes the most stringent Courant number condition because of small vertical grid spacing. Large Courant numbers are commonly found in regions where 1) bottom slope is large or; 2) shallow depths are discretized by multiple vertical layers. Therefore, we separate the vertical advection term from the other terms and solve it implicitly. Although some aspects of this approach have been presented elsewhere in the context of SCHISM's performance in the eddying regime (Zhang et al., 2016), we present the details of the new solver below for the sake of completeness.