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Developing Efficient High-Order Transport Schemes for Cross-Scale Coupled Estuary-Ocean Modeling

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DEVELOPING EFFICIENT HIGH-ORDER TRANSPORT SCHEMES
FOR CROSS-SCALE COUPLED ESTUARY-OCEAN MODELING

A Dissertation
Presented to
The Faculty of the School of Marine Science
The College of William and Mary in Virginia

In Partial Fulfillment
of the Requirements for the Degree of
Doctor of Philosophy

by
Fei Ye
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This dissertation is submitted in partial fulfillment of
the requirements for the degree of
Doctor of Philosophy

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<tr>
<td>Bay(^1) or CB</td>
<td>Chesapeake Bay</td>
</tr>
<tr>
<td>CBP</td>
<td>Chesapeake Bay Program</td>
</tr>
<tr>
<td>FE</td>
<td>Finite element</td>
</tr>
<tr>
<td>FV</td>
<td>Finite volume</td>
</tr>
<tr>
<td>GFD</td>
<td>Geophysical fluid dynamics</td>
</tr>
<tr>
<td>HPC</td>
<td>High performance computing</td>
</tr>
<tr>
<td>HYCOM</td>
<td>Hybrid Coordinate Ocean Model</td>
</tr>
<tr>
<td>NARR</td>
<td>North America Regional Reanalysis</td>
</tr>
<tr>
<td>NOAA</td>
<td>National Oceanic and Atmospheric Administration</td>
</tr>
<tr>
<td>SCHISM</td>
<td>Semi-implicit Cross-scale Hydroscience Integrated System Model</td>
</tr>
<tr>
<td>SG</td>
<td>Structured-grid</td>
</tr>
<tr>
<td>TVD</td>
<td>Total variation diminishing</td>
</tr>
<tr>
<td>UCB</td>
<td>Upper Chesapeake Bay</td>
</tr>
<tr>
<td>UG</td>
<td>Unstructured-grid</td>
</tr>
<tr>
<td>WENO</td>
<td>Weighted essentially non-oscillatory</td>
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\(^1\) When not associated with a name
Abstract

Geophysical fluid dynamics (GFD) models have progressed greatly in simulating the world’s oceans and estuaries in the past three decades, thanks to the development of novel numerical algorithms and the advent of massively parallel high-performance computing platforms. Study of inter-related processes on multi-scales (e.g., between large-scale (remote) processes and small-scale (local) processes) has always been an important theme for GFD modeling. For this purpose, models based on unstructured-grid (UG) have shown great potential because of their superior abilities in enabling multi-resolution and in fitting geometry and boundary. Despite UG models’ successful applications on coastal systems, significant obstacles still exist that have so far prevented UG models from realizing their full cross-scale capability. The pressing issues include the computation overhead resulting from large contrasts in the spatial resolutions, and the relative lack of skill for UG model in the eddying regime. Specifically for our own implicit UG model (SCHISM), the transport solver often emerges as a major bottleneck for both accuracy and efficiency.

The overall goal of this dissertation is two-fold. The first goal is to address the challenges in tracer transport by developing efficient high-order schemes for the transport processes and test them in the framework of a community supported modeling system (SCHISM: Semi-implicit Cross-scale Hydroscience Integrated System Model) for cross-scale processes. The second goal is to utilize the new schemes developed in this dissertation and elsewhere to build a bona fide cross-scale Chesapeake Bay model and use it to address some key knowledge gaps in the physical processes in this system and to better assist decision makers of coastal resource management.

The work on numerical scheme development has resulted in two new high-order transport solvers. The first solver tackles the vertical transport that often imposes the most stringent
constraint on model efficiency (Chapter 2). With an implicit method and two flux limiters in both space and time, the new TVD$^2$ solver leads to a speed-up of 1.6-6.0 in various cross-scale applications as compared to traditional explicit methods, while achieving 2nd-order accuracy in both space and time. Together with a flexible vertical gridding system, the flow over steep slopes can be faithfully simulated efficiently and accurately without altering the underlying bathymetry.

The second scheme aims at improving the model skill in the eddying ocean (Chapter 4). UG coastal models tend to under-resolve features like meso-scale eddies and meanders, and this issue is partially attributed to the numerical diffusion in the transport schemes that are originally developed for estuarine applications. To address this issue, a 3rd-order transport scheme based on WENO formulation is developed, and is demonstrated to improve the meso-scale features.

The new solvers are then tested in the Chesapeake Bay and adjacent Atlantic Ocean on small, medium and large domains respectively, corresponding to the three main chapters of this dissertation (Chapter 2-4), with an ultimate goal of achieving a seamless cross-scale model from the Gulf Stream to the shallow regions in the Bay tributaries and sub-tributaries. We highlight the dominant role played by the bathymetry in nearshore systems and the detrimental effects of bathymetric smoothing commonly used in many coastal models (Chapter 3). With the new methods developed in this dissertation and elsewhere, the model has enabled the analyses on some important processes that are hard to quantify with traditional techniques, e.g., the effect of channel-shoal contrast on lateral circulation and salinity distribution, hypoxia volume, the influence of realistic bathymetry on the freshwater plume etc. Potential topics for future research are also discussed at the end. In addition, the new solvers have also been successfully exported to many other oceanic and nearshore systems around the world via user groups of our community modeling system (cf. ‘Publications’ under ‘schism.wiki’).
Developing efficient high-order transport schemes for cross-scale coupled estuary-ocean modeling
1 Introduction

1.1 Motivation

Great progress has been made in simulating world’s oceans and estuaries in the past three decades and numerical models for GFD have become increasingly mature in their ability to hindcast past and forecast on-going and future changes in these systems. The combination of the advancement in numerical algorithms (Shchepetkin and McWilliams, 2005; Ringler et al., 2013; Wang et al., 2014; Chen et al., 2003; Luettich et al. 1992; Hamrick and Wu, 1997; Casulli and Cattani 1994; Fringer et al., 2006; Zhang and Baptista, 2008; Zhang et al., 2016a) and the advent of massively parallel HPC (High Performance Computing) infrastructure has dramatically increased the fidelity of modern GFD models.

Despite the progress, significant challenges remain in simulating cross-scale processes as commonly occurred in GFD. Cross-scale processes (CSP, aka multi-scale processes) are...
ubiquitous in world’s oceans and estuaries and rivers; e.g., the characteristic length of downward cascading meso-scale eddies toward the dissipation scales is reduced from hundreds of kilometers to <1 km (so-called sub-meso scale; Lévy et al., 2012). Figure 1-1 shows typical coastal and oceanic processes that span more than four order of magnitudes in time and space.

CSP are also very important for management purpose. Because the ‘local’ and ‘large’ scales are often intertwined, the coastal management has to not only assess the impact of their local practices on the large-scale systems, but also consider the influence of remote forcing from large scale processes on the local system. We illustrate two examples below that require a multi-scale integrated system approach:

1) Tsunami waves: typically a trans-oceanic event, it often generate highly heterogeneous coastal inundation hazards, as illustrated in Figure 1-2. This poses significant challenges for emergency management in planning/mitigation and evacuation during an event.

2) Migratory fishes: lifecycle of migratory fish species may cover a wide range of spatial scales (Norcross and Shaw, 1984); e.g., salmon are hatched in upstream rivers but spend the early life on the estuaries and continental shelf before returning to the spawning site as adults. This kind of fish movements are commonly modeled by an individual-based method, which depends on the simulated flow field (Werner et al., 2001). In this case, the most natural selection of a model domain is one that encompasses all of these pathways. After all, fish do not care about model boundaries any more than they care about jurisdictions by multiple agencies (the latter was commented by President Obama in his famous State of the Union speech in 2011). Artificially breaking up the connectivity of fish pathways into multiple sub-model domains can be problematic.
Figure 1-2: Spatial heterogeneity in coastal inundation during a 1993 tsunami event at Okushiri Island (Published by NOAA Center for Tsunami Research: https://nctr.pmel.noaa.gov/Pdf/okushiricolor.pdf).

Some knowledge gaps still exist in our understanding of cross-scale processes. For example, one of the on-going efforts in parameterizing turbulence mixing processes is to develop ‘scale-aware’ parameterization schemes for multi-scale applications that can mimic hydrostatic (at larger scales), non-hydrostatic (at medium scales) and LES (at small scales) (Luke van Roeke, private communication). However, even within the confine of the hydrostatic regime, current state-of-the-art numerical algorithms still need to be improved before they can effectively address the challenges associated with the significantly increased overhead in cross-scale simulating, a point alluded to in Danilov’s (2013) review of UG models. Traditionally, grid nesting technique is used for CSP, but it is not only cumbersome but also not seamless in terms
of boundary conditions and transitions across nests (Zhang et al., 2016b). This is both a practical issue and a fundamental issue. For example, Wolfe (2013) used San Francisco Bay as a case in point to expound the significance of the channel-shoal contrast as a fundamental process for estuarine dynamics, which has implication for stratification and spring blooms. A faithful representation of this contrast, however, requires higher resolution than most of the existing models can provide.

UG models have been demonstrated to be a promising candidate for simulating CSP due to their superior ability for local refinement/de-refinement and boundary-fitting; the latter is especially important in nearshore regime as the underlying geometry and bathymetry can be very complex. Recently, some UG models have also been shown to be more ‘science ready’ for CSP than the grid nesting approach using SGs (e.g., Ringer et al., 2013). Major challenges for applying UG models, especially in the large-scale eddying regime, have been succinctly summarized by Danilov (2013). In short, UG models are less efficient than their SG counterpart per degree of freedom due to the loss of cache efficiency as a result of ‘unstructuredness’ in the horizontal dimension; however, this is compensated by their flexibility in local refinement/de-refinement and the absence of land masking. Another challenge is related to the spurious numerical modes (Le Roux et al., 2005; Le Roux, 2012; Thuburn et al. 2009; Walters and Carey, 1983), which originate from the fact that the velocity space is larger than the pressure space (as dictated by the numerical stencil; Danilov 2013). This challenge had prevented UG models from being applied to large-scale eddying regime until recently, when it was overcome by either judicious design of the UG, numerical stencil and associated algorithm (e.g. in MPAS-OCEAN, Ringler et al., 2013) or intelligent stabilization schemes or filters (Danilov, 2013; Korn, 2017). Although UG models greatly extend the range of resolutions that can be covered by a GFD model, the separation between coastal and large-scale applications is likely to persist in the foreseeable future, due to the combination of very long time scale for the
global ocean to equilibrate and the prohibitively high CPU cost associated with higher resolution/larger grids (Danilov 2013).

Another important challenge for GFD models that has not received much attention so far is related to the bathymetry representation in a computational grid. This issue is of paramount significance in the nearshore regime as the bathymetry is one of the most fundamental forcings there and thus deserves much scrutiny. As we will demonstrate in Chapter 3, faithful representation of bathymetry (including topography in the inundation regime) is a must for nearshore models.

The challenges in CSP motivated us to develop novel algorithms and models that balance many competing considerations in building an ideal cross-scale model: accuracy (including accurate representation of the underlying bathymetry), efficiency, stability and robustness, and flexibility/extendibility. Currently we are restricting ourselves mostly in the hydrostatic regime but are making an effort to extend our models to non-hydrostatic regime. These considerations served to guide us in the evolution of our models from ELCIRC (Zhang et al., 2004) to SELFIE (Semi-implicit Eulerian–Lagrangian Finite-Element model; Zhang and Baptista, 2008) to SCHISM (Semi-implicit Cross-scale Hydroscience Integrated System Model; Zhang et al., 2016a). This dissertation builds on the SCHISM modeling system by addressing some critical challenges in simulating CSP. A main goal is to develop advanced numerical methods within the SCHISM modeling system, and apply them in building a 3D baroclinic model for the Chesapeake Bay and the adjacent Atlantic Ocean. We chose SCHISM here because some of its characteristics are ideal for CSP: (1) the use of generic (non-orthogonal) unstructured grids provides maximum flexibility in field applications; (2) implicit time stepping bypasses most stringent stability constraints and thus allows users to focus more on physics rather than numerics; (3) a novel and highly flexible vertical gridding system allows a seamless transition from eddying to non-eddying regimes, while faithfully preserving the original bathymetry.
However, even with these features of SCHISM in place several years ago, we found that one of the key bottlenecks in building a bona fide cross-scale model is the transport solver, which will be the focus of this dissertation.

1.2 The testbed of the new methods developed in this dissertation

The primary application site of this dissertation, the Chesapeake Bay, serves as a good testbed for the model’s cross-scale capability due to its complex geometry and bathymetry, as well as its highly variable stratification. The Bay processes are closely linked to both the small-scale processes occurring in the tributaries/sub-tributaries and the large-scale processes in the coastal ocean such as the Gulf Stream (Schubel and Pritchard, 1986; Goodrich et al., 1987; Valle-Levinson and Lwiza, 1997; Ezer, 2013; Nicholls et al., 2007); the proper investigation of these processes requires cross-scale modeling capability.

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 fate under climate change (Hagy et al., 2004; Najjar et al., 2010; Murphy et al., 2011; Hong and Shen, 2012). In recent years, more and more focus has been placed on its productive tributaries and shallow regions, which have drawn particular interest from management (Cerco et al., 2013). As in other estuarine and coastal systems, 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).
As an intensively studied estuary in the US, the Chesapeake Bay has seen plenty of modeling activities since the 1960s (Boicourt, W., 1969). At the whole-bay level, 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 was also included in the Chesapeake Bay model inter-comparison conducted by NOAA (Irby et al., 2016). This inter-comparison demonstrated that all participating models (mainly based on SGs with the exception of FVCOM) 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, due to the lack of resolution there. The limited cross-scale capability of the structured-grid models led to insufficient resolutions in the shallows and tributaries (Cerco et al., 2013). Moreover, bathymetry smoothing or regularization (in order to capture the effective volume) is commonly applied in models, especially those based on terrain-following coordinates, which often artificially enhances the simulated salt intrusion. However, the mismatch in bathymetry can impair the applicability of the models in certain cases. For example, the volume of water below pycnocline (which is highly correlated with hypoxia volume) can be misinterpreted. In addition, the interaction between the Bay, tributaries, and the coastal ocean are understudied by numerical models, as pointed out by Jiang and Xia (2016). Many cross-scale processes and their implications on the Bay are not well understood at the moment. These include (but are not limited to) the effects of the coastal upwelling/downwelling events and large-scale processes such as the Gulf Stream on estuarine circulation (Ezer, 2013; Ryan et al., 2001). Therefore, an efficient and accurate cross-scale model is highly desirable for testing hypotheses that relate tributary and Bay scale dynamics to large-scale processes.

1.3 Dissertation objectives and structure
The overarching goal of this dissertation is two-fold: (1) developing new numerical methods for the transport solver to improve the cross-scale capability of our UG coastal model in terms of accuracy and efficiency; and (2) applying these techniques in constructing a bona fide cross-scale Chesapeake Bay model to assist decision making by qualitatively and quantitatively assessing some interrelated processes occurring on contrasting spatial and temporal scales.

The development work of this dissertation has resulted in two new high-order transport solvers for vertical and horizontal dimensions respectively. The first solver improves efficiency (by a factor of 1.4-6.0 in various applications tested so far) as well as accuracy; the second solver enhances model’s eddy-resolving capability in the eddying regime. These new developments enable us to simulate coastal processes more accurately and more efficiently on a wider range of spatial and temporal scales. The details of the numerical techniques will not be presented in stand-alone chapters mainly for the sake of compactness; instead, they are presented in the context of specific applications in small, medium, and large domains (Chapter 2, 3, & 4 respectively). These applications serve as building blocks toward our ultimate goal of developing a seamless cross-scale model that covers the Chesapeake Bay system from its sub-tributaries to the Gulf Stream. They have also served as baseline models for many interdisciplinary studies, e.g., in several biological and water quality studies in the Chesapeake Bay (Zhang and Wang, 2016) and in the decision support on a few proposed engineering projects (Liu et al. submitted; Ye et al., submitted).

Chapter 2 deals with a key bottleneck that prevents our UG model from realizing its full potential in cross-scale modeling: the efficiency loss in the transport solver due to large variations in grid resolution. The starting hypothesis was that the efficiency/accuracy of the transport solver can be improved by nonlinear implicit time stepping in the vertical dimension, which is proved by a previous theoretical study, our numerical benchmarks and a real application in the Upper Chesapeake Bay. In addition, the method has been applied and
validated in many other systems over the world (Zhang et al., 2016a; Yu et al., 2017) as well as in the challenging case of the CB and its adjacent coastal ocean (Chapter 3). This chapter is adapted from a paper published in Ocean Modelling (Ye et al., 2016).

**Chapter 3** addresses a very important topic in the nearshore regime, i.e. the bathymetry errors in models. We first develops a cross-scale model for the CB, which distinguishes from other Bay models in two key aspects: (1) it adopts a flexible vertical grid design of LSC$^2$ (Zhang et al., 2015), which faithfully represents bathymetry *without any smoothing*, at the same time reducing unphysical diapycnal mixing and pressure gradient error as commonly associated with terrain-following coordinates; (2) it utilizes the implicit transport solver developed in the previous chapter, which enables accurate and efficient baroclinic simulations on a large domain with local refinements targeted at any sub-regions of interest; these features are highly desirable for management purpose, since productive tributaries and shallow regions are of particular interest, and our model represents a holistic approach that includes both local and remote forcings. These new features also facilitate a systematic investigation on the effect of bathymetry smoothing commonly practiced in terrain-following coordinate models. We show that bathymetry smoothing leads to fundamental, systemic changes with respect to circulation patterns (e.g. channel-shoal contrasts), bottom stress (important for sediment transport), turbulence mixing, and volumetric/tracer fluxes. Therefore, bathymetry smoothing should be avoided in general. This chapter is adapted from a paper submitted to Ocean Modelling and under revision (Ye et al, in revision).

**Chapter 4** focuses on enhancing the model’s performance in the eddying ocean. This is partially motivated by the work in Chapter 3, where errors and uncertainties in the ocean boundary conditions are found to adversely influence the simulated estuarine dynamics. The large-scale processes (e.g., the fluctuations and shelf intrusions of the Gulf Stream) can affect small-scale local systems, and therefore need to be properly represented in a cross-scale model.
However, the transport schemes that are considered sufficient in an estuarine setting are shown to be diffusive for the eddying regime. To fill in this gap, a 3rd order transport scheme based on Weighted Essentially Non- Oscillatory (WENO) formulation is developed for the horizontal tracer transport on an unstructured triangle-quadrangle grid, and is applied to the Atlantic Ocean along the US east coast. The new scheme is shown to improve the meso-scale eddying and meandering processes that are commonly observed near the Gulf Stream, thus ideal for cross-scale applications.

A brief summary of major findings in this dissertation and potential future research areas is presented in Chapter 5.
2 Small domain: A 3D, cross-scale, baroclinic model with implicit vertical transport for the Upper Chesapeake Bay and its tributaries

(Adapted from Ye et al., Ocean Modelling, 107, pp.82-96. doi: 10.1016/j.ocemod.2016.10.004)

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.

Keywords: cross-scale, SCHISM, estuarine circulation, implicit transport, Chesapeake Bay, USA
2.1 Introduction

As discussed in Chapter 1, there is 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. An inter-comparison of models was 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 because 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 and is also cumbersome for complex geometry.

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. (2016a), 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., 2016a). 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 1-D 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., 2016a) 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 (cf. Figure 4-1 in Chapter 4) 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 then proceed to applying the same technique to a seamless shelf-bay-tributary model that covers the whole Bay and extends beyond the continental slope in Chapter 3. 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 2.2), and then describe the set-up (Section 2.3) and
validation (Section 2.4) of the UCB model. The sensitivity and cross-scale capability of the UCB model are discussed in Section 2.5, followed by conclusions in Section 2.6.

2.2 New transport solver

2.2.1 Formulation

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

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

(2.1)

where \( T \) represents the concentration of a generic tracer; \( \kappa \) 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 (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.
Based on a finite-volume discretization (Figure 2-1), we write the transport equation Eq. (2.1) in a semi-discretized form:

\[
T_i^{n+1} - T_i^n = -\frac{\Delta t}{V_i} \left[ \sum_{j \in S^+} (|Q_j| T'_j) - \sum_{j \in S^-} (|Q_j| T'_j) \right] \\
+ \frac{\Delta t}{V_i} \left[ \left( \kappa'_j \frac{\partial T_i}{\partial z} \right)_{j=i\cap i^+} - \left( \kappa'_j \frac{\partial T_i}{\partial z} \right)_{j=i\cap i^-} \right] + \frac{\Delta t}{V_i} \int q,
\]

where \(T\) is concentration defined at prism centers (or more precisely, average concentration in a prism); \(T'\) is concentration at a face of the prism, which will be reconstructed from prismatic concentration \(T\) in subsequent steps; \(i\) is a prism index; \(j\) is a face index; \(n\) is time level; \(V_i\) is the volume of Prism \(i\); \(Q\) (positive leaving Prism \(i\)) is the volumetric flux through faces, which has already been solved by the momentum equation at the current step; \(\kappa'\) is vertical diffusivity defined at top or bottom faces of the prism. \(S\) denotes all prism faces including inflow faces \(S^-\) and outflow faces \(S^+\). Additional symbols of vertical levels are introduced for convenience: \(i^+\) is the prism on top of Prism \(i\); \(i^-\) is the prism below Prism \(i\); \(i \cap i^+\) is the top face of Prism \(i\); \(i \cap i^-\) is the bottom face of Prism \(i\). The time levels of \(T\) on the right-hand side (RHS) of Eq. (2.2) will be specified next.
To facilitate operator splitting, we write the reconstructed face concentration in the form of an upwind reconstruction plus a correction term to achieve higher order:

\[ T_j' = T_{\text{up}} + \Phi_j, \]  

or

\[
\begin{cases} 
T_j' = T_{je} + \Phi_j, & j \in S^- \\
T_j' = T_i + \Phi_j, & j \in S^+ 
\end{cases}
\]  

where \( T_{je} \) is the element sharing side \( j \) with element \( i \); \( \Phi \) is the corrections applied on the upwind flux, which can take different forms in different schemes. Also, in the following text, \( T_{je} \) will be abbreviated as \( T_j \), with the understanding that \( T_j \) is prism concentration and different from the side concentration \( T_j' \) (with the prime symbol signifying side-based values). Using equation (2.4), equation (2.2) can be written as:

\[
\tau_{i+1} - \tau_i = \frac{\Delta t}{V_i} \left[ \sum_{j \in S^+} (|Q_j|T_i) - \sum_{j \in S^-} (|Q_j|T_j) + \sum_{j \in S^+} (|Q_j|\Phi_j) - \sum_{j \in S^-} (|Q_j|\Phi_j) \right]
\]  

(2.5)
\[ + \frac{\Delta t}{V_i} \left[ \left( \kappa'_j \frac{\partial T_j}{\partial z} \right)_{j = i \cap i^+} - \left( \kappa'_j \frac{\partial T_j}{\partial z} \right)_{j = i \cap i^-} \right] + \frac{\Delta t}{V_i} \int q \]

Note that the first term on the R.H.S. can be rewritten as

\[ \sum_{j \in S^+} (|Q_j| T_i) \equiv \left( \sum_{j \in S^+} |Q_j| \right) T_i = \left( \sum_{j \in S^-} |Q_j| \right) T_i \equiv \sum_{j \in S^-} (|Q_j| T_i), \quad (2.6) \]

which is possible because (i) \( T_i \) is independent of the summations \( \sum_{j \in S^+} \sum_{j \in S^-} \); and (ii) the volume conservation \( \sum_{j \in S^+} |Q_j| = \sum_{j \in S^-} |Q_j| \) is guaranteed by the FV solver for the vertical velocity used in SCHISM. Using Eq. (2.6), Eq. (2.5) can be written as

\[ T_i^{n+1} - T_i^n = -\frac{\Delta t}{V_i} \left\{ \sum_{j \in S_H} \left[ |Q_j| (T_i - T_j) \right] + \sum_{j \in S_H^v} \left[ |Q_j| \Phi_j \right] - \sum_{j \in S_H^b} \left[ |Q_j| \Phi_j \right] \right\} \]

\[ + \frac{\Delta t}{V_i} \left[ \left( \kappa'_j \frac{\partial T_j}{\partial z} \right)_{j = i \cap i^+} - \left( \kappa'_j \frac{\partial T_j}{\partial z} \right)_{j = i \cap i^-} \right] + \frac{\Delta t}{V_i} \int q. \quad (2.7) \]

We solve the discretized transport equation (2.7) in three steps: horizontal advection, vertical advection, and vertical diffusion plus other terms. Each step deals with different terms on the RHS of (2.7):

**Step 1**

Horizontal advection

\[ T_i^{(1)} - T_i^n = -\frac{\Delta t}{V_i} \left\{ \sum_{j \in S_H} \left[ |Q_j| (T_i - T_j) \right] + \sum_{j \in S_H^v} \left[ |Q_j| \Phi_j \right] - \sum_{j \in S_H^b} \left[ |Q_j| \Phi_j \right] \right\}, \quad (2.8) \]

**Step 2**

Vertical advection

\[ T_i^{(2)} - T_i^{(1)} = -\frac{\Delta t}{V_i} \left\{ \sum_{j \in S_H^v} \left[ |Q_j| (T_i - T_j) \right] + \sum_{j \in S_H^b} \left[ |Q_j| \Phi_j \right] - \sum_{j \in S_H^b} \left[ |Q_j| \Phi_j \right] \right\}, \quad (2.9) \]

**Step 3**

Vertical diffusion and source

\[ T_i^{n+1} - T_i^{(2)} = \frac{\Delta t}{V_i} \left[ \left( \kappa'_j \frac{\partial T_j}{\partial z} \right)_{j = i \cap i^+}^{n+1} - \left( \kappa'_j \frac{\partial T_j}{\partial z} \right)_{j = i \cap i^-}^{n+1} \right] + \frac{\Delta t}{V_i} \int q, \]
where $T^{(1)}$ is the horizontally advected concentration; $T^{(2)}$ is the horizontally and vertically advected concentration; $S_H$ denotes all vertical faces of prism $i$; $S_V$ denotes the top and bottom faces of prism $i$. The details of this procedure are described below, with emphasis on Step 2 that involves the vertical advection and the implicit TVD scheme.

**Step 1: horizontal advection**

Previously, the horizontal advection in SCHISM was solved by an explicit 2nd-order TVD scheme, which is proved sufficient for estuarine applications but not for the eddying ocean. We will come back to this issue in Chapter 4, where a 3rd-order scheme is developed; for the time being, the traditional TVD formulation is presented here. Starting from time level $n$ and using approximated face values, Eq. (2.8) is solved explicitly through sub-cycling:

$$T_i^{m+1} = T_i^m + \frac{\Delta t_m^i}{V_i} \sum_{j \in S_H} Q_j |T_j^m - T_i^m| - \frac{\Delta t_m^i}{V_i} \sum_{j \in S_H} |Q_j| \sigma_j^{m},$$

(2.11)

where $m = 1, \ldots, M$ is the index of sub-steps; $\Delta t_m^i$ is the sub-time step of each sub-cycle subjected to the horizontal Courant number condition; $T_i$ is the concentration of prism $i$; $T_j$ is the concentration of the prism that shares face $j$ with element $i$. Note that without the last term, Eq. (2.11) is an upwind scheme with the inflow face concentration approximated by $T_j$ and the outflow face concentration by $T_i$. Also note that the last term in Eq. (2.11) is the combination of the last two terms in Eq. (2.8) and the generic correction term $\Phi$ is materialized with the TVD limiter term $\sigma$ to achieve 2nd-order accuracy, for which the standard choice of limiter functions can be used (Sweby 1984). At the last sub-cycle $m=M$, we obtain the horizontally advected concentration $T_i^{(1)} \equiv T^{M+1}$. The number of horizontal sub-cycle $M$ is determined globally by the most restrictive element. This is tolerable in terms of maintaining the efficiency.
of the transport solver, because the horizontal Courant condition is generally much less restrictive than the vertical Courant condition in realistic applications. In the case of very high horizontal resolution locally, the model allows the use of upwind scheme in lieu of TVD, as the former is sufficiently accurate with the high resolution.

**Step 2: vertical advection**

Starting from the horizontally advected concentration $T_i^{(1)}$, the vertical advection is solved iteratively using the finite-volume implicit TVD (TVD$^2$) scheme. The superscript ‘2’ refers to the direct second-order reconstruction of face values $T'$ in both space and time with two TVD limiters. The idea was first suggested by Duraisamy and Baeder (2007) in their *implicit second-order space-time reconstruction* scheme. The reconstructed face value is obtained through the following Taylor series expansion in space and time:

$$T_j' = T_{jU}^{(2)} + \frac{1}{2} \frac{H_{jU}}{z_{jD} - z_{jU}} (T_{jD}^{(2)} - T_{jU}^{(2)}) - \frac{1}{2} (T_{jU}^{(2)} - T_{jU}^{(1)}),$$

where $jU$ and $jD$ are the upwind and downwind prisms of face $j$ respectively; $H$ is prism height; $z$ is the vertical coordinate of prism centers. Note that $T^{(2)}$ is to be solved implicitly. Introducing the space TVD limiter $\phi$ and the time limiter $\psi$ on the two central difference terms on the RHS of Eq. (2.12) in order to guarantee monotonicity, we have:

$$T_j' = T_{jU}^{(2)} + \frac{\phi_j}{2} (T_{jD}^{(2)} - T_{jU}^{(2)}) - \frac{\psi_j}{2} (T_{jU}^{(2)} - T_{jU}^{(1)}).$$

We have made the simplification $\frac{H_{jU}}{z_{jD} - z_{jU}} \approx 1$ on the spatial reconstruction term of Eq. (2.13), and tacitly assume that $\phi_j = 1$ corresponds to a central difference. This essentially sacrifices some accuracy on non-uniform grids, but greatly simplifies the TVD condition. Note that Eq. (2.13) is consistent with the generic formulation of Eq. (2.3). Substituting the reconstructed face value $T'$ from Eq. (2.13) into the discretized vertical advection equation (2.9), we have:
\[ T_i^{(2)} + \frac{\Delta t}{V_i} \sum_{j \in S_i^+} |Q_j| (T_i^{(2)} - T_j^{(2)}) \]
\[ + \frac{\Delta t}{V_i} \sum_{j \in S_i^+} \frac{1}{2} |Q_j| \phi_j (T_j^{(2)} - T_i^{(2)}) - \frac{\Delta t}{V_i} \sum_{j \in S_i^+} \frac{1}{2} |Q_j| \phi_j (T_i^{(2)} - T_j^{(2)}) \]
\[ - \frac{\Delta t}{V_i} \sum_{j \in S_i^+} \frac{1}{2} |Q_j| \psi_j (T_i^{(2)} - T_j^{(1)}) + \frac{\Delta t}{V_i} \sum_{j \in S_i^+} \frac{1}{2} |Q_j| \phi_j (T_i^{(2)} - T_j^{(1)}) = T_i^{(1)}. \] (2.14)

Note that \( jU \) in Eq. (2.13) does not appear in Eq. (2.14). This is because face \( j \)'s upwind prism is either prism \( i \) or the neighbor of prism \( i \), and can be determined by the flux direction at face \( j \). The same applies to \( jD \). In order to make Eq. (2.14) more compact for deriving the TVD condition and coding, we introduce the upwind ratio \( r \) and the downwind ratio \( s \) defined on faces:

\[ r_j = \frac{\sum_{p \in S_i^+} |Q_p| (T_p^{(2)} - T_i^{(2)})}{|Q_j| (T_j^{(2)} - T_i^{(2)})}, (j \in S_i^+), \] (2.15)
\[ s_j = \frac{\sum_{p \in S_i^+} |Q_p| (T_i^{(2)} - T_p^{(1)})}{|Q_j| (T_j^{(2)} - T_i^{(1)})}, (j \in S_i^+). \]

At the free surface and bottom, \( r \) and \( s \) are set to 0. With these ratios, Eq. (2.14) can be written as

\[ T_i^{(2)} + \frac{\Delta t}{V_i} \sum_{j \in S_i^+} |Q_j| (T_i^{(2)} - T_j^{(2)}) \]
\[ + \frac{1}{2} \frac{\Delta t}{V_i} \sum_{j \in S_i^+} \left[ \left( \sum_{p \in S_i^+} \phi_p r_p - \phi_j \right) |Q_j| (T_i^{(2)} - T_j^{(2)}) \right] \]
\[ + \frac{1}{2} \frac{\Delta t}{V_i} \sum_{j \in S_i^+} \left[ \left( \sum_{p \in S_i^+} \psi_p r_p - \psi_j \right) |Q_j| (T_i^{(2)} - T_j^{(1)}) \right] = T_i^{(1)}, \] (2.16)

which can be further simplified to:
\[ T^{(2)}_i + \frac{\Delta t}{V_i} \sum_{j \in S_Y} \left( |Q_j| \left[ 1 + \frac{1}{2} \left( \sum_{p \in S_Y} \frac{\phi_p}{r_p} - \phi_j \right) \right] \left( T^{(2)}_i - T^{(2)}_j \right) \right) \]
\[ = T^{(1)}_i \]
\[ (2.17) \]

Since a prism only has two faces in the vertical dimension, Eq. (2.17) could be easily assembled into a tri-diagonal matrix. However, Eq. (2.17) cannot be solved directly because the coefficients \( \phi \), \( \psi \), \( r \), and \( s \) are non-linear, so an iterative method is necessary. With the coefficients being evaluated at the previous iteration, Eq. (2.17) can be linearized and solved iteratively as:

\[ T^{S+1}_i + \frac{\Delta t}{V_i} \sum_{j \in S_Y} \left( |Q_j| \left[ 1 + \frac{1}{2} \left( \sum_{p \in S_Y} \frac{\phi_p^S}{r_p} - \phi_j^S \right) \right] \left( T^{S+1}_i - T^{S+1}_j \right) \right) \]
\[ = T^{S}_i \]
\[ (2.18) \]

\[ (T^{S}_i = T^{(1)}_i \text{ for the first iteration}), \]

where \( s \) is the index of nonlinear iterations. We obtain the horizontally and vertically advected concentration \( T^{(2)}_i \equiv T^{S+1}_i \) upon convergence, i.e., when:

\[ \sqrt{\sum_{i=1}^{n_v} (T^{S+1}_i - T^{S}_i)^2} \leq \epsilon_1 \sqrt{\sum_{i=1}^{n_v} (T^{S}_i)^2} + \epsilon_2, \]
\[ (2.19) \]

where \( n_v \) is the number of vertical layers; \( \epsilon_1, \epsilon_2 \) are small positive numbers. In realistic applications, we choose \( \epsilon_1 \) in the range of \( 10^{-9} \sim 10^{-4} \), and \( \epsilon_2 = 10^{-14} \), and fast convergence within a few iterations is usually observed.

Although this concludes the solution procedure, we further provide the proof of monotonicity and the appropriate forms of limiters. Harten and Lax (1984) proved that a sufficient condition for the scheme \( T^{S+1}_i + \sum_{j \in S_Y} C_j \left( T^{S+1}_i - T^{S+1}_j \right) = T^{S} \) to be TVD is \( C_j \geq 0 \) (\( j \in S_Y \)). The symbols follow the convention in this paper, and the original form can be found in Lemma 3.2 of Harten and Lax (1984). Therefore, the TVD condition for Eq. (2.18) is:
\[ 1 + \frac{1}{2} \left( \sum_{p \in S_{j}^-} \phi_p^s \frac{s_p^s}{r_p^s} - \phi_j^s \right) \geq 0, \quad (j \in S_{j}^-) \]  

(2.20)

and

\[ 1 + \frac{1}{2} \Delta t \sum_{j \in S_{j}^+} |Q_j| \left( \sum_{p \in S_{j}^+} \psi_p^s \frac{s_p^s}{s_p^s} - \psi_j^s \right) > 0. \]

(2.21)

Eq. (2.20) is automatically satisfied with any choice of standard TVD limiters in space (Sweby, 1984). To derive the TVD condition for (2.21), we need to consider three types of vertical flows that can occur at a given prism: uni-directional, convergent, or divergent.

(i) Under the uni-directional flow, both \( S_{j}^+ \) and \( S_{j}^- \) are present. Eq.(2.21) reduces to

\[ 1 + \frac{1}{2} \frac{\Delta t |Q_j|}{V_i} \left( \frac{\psi_j^s}{s_p^s} - \psi_j^s \right) > 0, \quad (p \in S_{j}^-, j \in S_{j}^+), \]

which is satisfied by

\[ \psi_j = \max \left\{ 0, \min \left[ 1, \frac{2V_i}{\Delta t |Q_j|} \cdot (1 - \epsilon_3) \right] \right\}, \quad j \in S_{j}^+. \]

(2.22)

where \( \epsilon_3 \) is a small positive number. This time limiter formulation is slightly different from Duraisamy and Baeder (2007)’s. Our benchmarks and real estuary applications showed the time limiter specified by Eq. (2.22) slightly reduces numerical diffusion. Eq. (2.18) and Eq. (2.22) are then iteratively solved. Note that \( \psi_j \) in Eq. (2.22) is defined on faces and dependent on its upwind prism \( i \). There are two special cases where the upwind prism of a face is undefined at the boundaries: falling free surface and rising bottom (although the latter rarely occurs in practice). In these cases, \( \psi_j \) is set to 0.

(ii) Under convergent flows, \( S_{j}^+ \) vanishes. Eq. (2.21) is always satisfied because the outer sum vanishes.

(iii) Under divergent flows, \( S_{j}^- \) vanishes. Eq. (2.18) reduces to \( T_i^{s+1} = T_i^s \), and no limiters need to be evaluated.
**Step 3: vertical diffusion and source**

The vertical diffusion and source terms are also solved implicitly as:

\[
T_i^{n+1} = T_i^{(2)} + \frac{\Delta t}{V_i} \left[ \kappa'_{i,n(i+1)} \frac{T_i^{n+1} - T_i^{n+1}}{z_{i+1} - z_i} - \kappa'_{i,n(i-1)} \frac{T_i^{n+1} - T_i^{n+1}}{z_i - z_{i-1}} \right] + \frac{\Delta t}{V_i} \int q_i^{n+1}. \tag{2.23}
\]

Note that the source terms are usually known. The vertical diffusion and other terms are separated from the vertical advection because the boundary condition of these terms may compromise the TVD property in Step 2. Moreover, since Eq. (2.23) can be written as a linear tri-diagonal system that is easily solved without sub-cycling, we did not combine Step 3 with Step 1. In practice, the time step \( \Delta t \) of the implicit solvers in Steps 2 and 3 is the same as the main model time step.

### 2.2.2 Numerical benchmark

Our work is an extension of Duraisamy and Baeder (2007)’s scheme into more complex 3D flows typically found in an estuary and ocean setting. We will not duplicate their 1-D numerical tests for the advection under a constant velocity with no boundary conditions; the readers can find the relevant 1-D tests in Figure 2-3 in Duraisamy and Baeder (2007) and Figure 2-5 in Norouzi and Timofeev (2011). The general conclusion was that the implicit TVD scheme with temporal/spatial limiters is less diffusive than traditional implicit schemes, and even than the explicit TVD scheme where the time step of the explicit scheme is constrained by large variations in element size.

Since our main contribution is the treatment of complex flow patterns (non-constant, divergent, and convergent), as well as the treatment of surface and bottom boundary conditions for a typical ocean model, we choose the lock exchange test (Ilicak et al., 2012) to compare the numerical diffusion introduced by the explicit and implicit TVD solvers in a hydrodynamic setting. The test domain is a rectangular box of 64 km long and 20 km wide, with a uniform
depth of 20 m. Initially, the water is at rest, with a uniform temperature of 5 °C in the left half of the domain and a uniform temperature of 35 °C in the right half, with \( x=0 \) being the division line. Once the two water bodies start to mix, the density driven flow generates a pycnocline in the middle layers, as well as two fronts traveling in opposite directions (Figure 2-2). An analytical solution is available for the propagation speed of this gravity current (Benjamin, 1968). Since the analytical solution represents an ideal case with no physical mixing, the numerical diffusion of the two solvers can be examined. In this test, the horizontal domain is discretized with a uniform resolution of 500 m, and the vertical dimension consists of 20 evenly spaced sigma layers with 1 m thickness initially. A time step of 150 seconds is used. The resolution and time scales in this set-up resemble those typically found in a real estuary application. The simulation is run for 17 hours, until the two fronts almost reach the boundary.

Figure 2-2: Numerical results of the simulated lock exchange problem at \( t = 17 \) h, with \( \Delta t = 150 \) s: (a) explicit TVD solver; (b) implicit TVD solver. The vertical transect is along the center line of the domain.
The results from both solvers (Figure 2-2) show thinner pycnoclines compared to some other models (Ilıcak et al., 2012). With both solvers, the simulated fronts slightly lag behind the analytical solution (Figure 2-3), indicating the presence of numerical diffusion. Analytically, the surface and bottom fronts should reach \( x = \pm 29.92 \text{ km} \) after 17 hours, which translates to an average frontal speed of 1.76 \( \text{km h}^{-1} \). The relative error of the frontal speed is 4.46% with the explicit solver, and 3.35% with the implicit solver. In addition, the implicit solver reduces the computational cost by 4.5%. Although the improvement from the implicit solver is relatively modest in this simple benchmark (as well as in the 1-D benchmarks done by others), it becomes much more evident in real applications as discussed later (Section 2.5.1).

![Figure 2-3: Time history of the analytical and simulated frontal locations in the lock exchange problem, with the left panel showing the whole time history, and the right panel showing the last 2 hours.](image)

### 2.3 The Upper Chesapeake Bay model

We apply three recently developed techniques to our UCB implementation, including the FV-TVD\(^2\) scheme presented in Section 2.2, the mixed quad/triangle mesh (Zhang et al., 2016a), and the localized sigma coordinates with shaved cell (LSC\(^2\); Zhang et al., 2015). These techniques ensure both accuracy and efficiency in the simulated cross-scale processes, and
distinguish our UCB model from previous modeling studies of the Bay. In this section, we first review the data available for model validation and describe the model forcing and set-up.

2.3.1 The Upper Bay model domain and available observations

Our UCB domain extends northward from Solomons Island, Maryland to the downstream part of the Susquehanna River (Figure 2-4). The Susquehanna River delivers 87% of the total freshwater discharge to the UCB (Schubel and Pritchard, 1986), and is the major driver of stratification. Other freshwater inputs included in the model are: 1) the second largest river in the model domain, Choptank River; 2) the local areas of interest, Baltimore Harbor and Chester River. The UCB domain is mostly shallow, but with a deep main shipping channel of 20-40 m (Figure 2-4). The channel bifurcates near Sandy Point (39° 01' N, 76° 23' W), with one branch continuing along the bay main stem, and the other branch (Craighill Channel) turning into the Baltimore Harbor and joining the Brewerton Channel. This deep channel leads to some unique circulation and salinity patterns in Baltimore Harbor as will be described later in Section 2.5.3. We will also study another tributary, the Chester River (including its sub-tributary the Corsica River), because: 1) it is a relatively large tributary in the model domain; 2) it has complex channel shapes and bathymetry; 3) it is subjected to large salinity variations at the mouth, due to its proximity to the Susquehanna River. These features put a stringent test on the model’s cross-scale capability and we will demonstrate that the implicit solvers inside SCHISM are critical in resolving those features at a minimal cost. Moreover, the water quality of the Chester River and other shallow regions is of management interest, and thus a tributary-resolving water quality model is desirable (Zhang and Wang, 2016). In this case, the transport solver must be efficient when downscaling into this region, because over twenty water quality variables need to be calculated.
Four types of observed data are used for validation: 1) 6-min free-surface elevation from NOAA tidal gauges; 2) 6-min vertical velocity profiles from a NOAA ADCP; 3) monthly or bi-weekly salinity/temperature profiles from the CBP Water Quality Database (http://www.chesapeakebay.net/data/downloads/cbp_water_quality_database_1984_present, last accessed on Sept. 10, 2015); 4) 15-min surface/bottom salinity from Maryland Eyes on the Bay’s continuous monitoring (CMON) database (http://mddnr.chesapeakebay.net/eyesonthebay/index.cfm, last accessed on Sept. 10, 2015).

The locations of the sampling stations are shown in Figure 2-4a. The bathymetry is from NOAA (http://www.ngdc.noaa.gov/mgg/gdas/gd_designagrid.html, last accessed on Oct. 13, 2013).

2.3.2 Model forcings
The primary simulation period is from June 1, 2003 to Dec 31, 2004. We chose this period because a high-quality atmospheric product exists only during this period: a hybrid wind dataset blending North American Regional Reanalysis (NARR) and NOAA observations made available from a previous work (Lanerolle et al., 2011). Compared to the pure NARR wind, the hybrid wind possesses more spatial/temporal variability and gusts. As will be shown in Section 2.5.2, the use of the hybrid product leads to a more realistic wind-induced mixing. The primary simulation period includes some typical variability of the flow regime: a portion of a wet year 2003, a less wet year 2004, and one extreme event (Hurricane Isabel in September 2003). In addition, we also carried out a longer 2003~2011 simulation with an identical set-up except that the unmodified NARR wind was used. This serves as a supplement for model validation in a few cases where observations are not available in the primary simulation period. Other atmospheric forcing applied at the surface is taken from NARR, including: atmospheric pressure (important during storms), downward short-wave and long-wave radiation fluxes, air temperature, specific humidity, and precipitation. The effect of direct precipitation is found to be negligible.

Along the downstream (southern) boundary, the imposed elevation comes from observations at the NOAA station Solomons Island (8577330). Cross-channel differences are neglected because the boundary is relatively narrow. The salinity and temperature along this transect are specified by the observations at the CBP station CB4.4 located at 4 km upstream of the boundary (Figure 2-4a). The bi-weekly/monthly observed vertical profiles are applied across the entire boundary, with a spatial interpolation based on depth, and a linear interpolation in time. The salinity and temperature from the downstream boundary to CB4.4 are strongly nudged to the boundary condition in order to generate an exchange flow, because the velocity boundary conditions are lacking.
Imposed at the upstream (riverine) boundaries are observed daily mean discharges at two USGS stations: 01578310 Susquehanna River at Conowingo, MD; 01491000 Choptank River near Greensboro, MD, where salinity is set to zero. The water temperature is interpolated in time from the monthly observations at the closest CBP stations (CB1.1 for Susquehanna; ET5.1 for Choptank). The watershed inflows along the land boundaries of the UCB main stem and most tributaries are neglected, as sensitivity tests show they have little effect on the UCB main stem. However, we prescribe lateral inflows for Baltimore Harbor and Chester River with the point and non-point sources from CBP’s Phase 5.3.2 community watershed model (http://ches.communitymodeling.org/models/CBPhase5/documentation.php, last accessed on Oct. 2, 2015) in order to demonstrate the cross-scale capability of our model, because freshwater inputs in these tributaries influence the results locally.

Initially the water is at rest. The initial 3D salinity/temperature field is based on the observations at CBP stations along the main shipping channel (Figure 2-4). Salinity and temperature are first interpolated along the longitudinal transect, and then horizontally extrapolated in the cross-channel direction at each depth. Since the mean residence time in the modeled region is about 3 months, as estimated from a mean flow year (Hong and Shen, 2012), and at most 4 months in the dry period (Du and Shen 2016), the model is considered adequately spun up before Hurricane Isabel in late September, 2003.

2.3.3 Model set-up

The model grid consists of 26,027 elements (including both triangles and quadrilaterals) and 16,374 nodes in the horizontal, and an average of 23.5 vertical layers (locally varying between 1 and 50 levels). The quadrilaterals are used in the main channel of the Upper Bay and minor tributaries that only require 2D or 1D representation; the triangles are used in other areas. The rationale for using a mixed grid is that pure quadrilaterals are better suited to model channelized
flow (Rayson et al. 2015) and more economical (as the number of elements is halved compared to triangles) but are unable to resolve the complex shoals, whereas triangles are capable of resolving complex geometry, but are less ideal for channelized flow and are also less economical. The mixed grid effectively takes full advantage of a structured grid within an unstructured-grid framework. In general, the grid resolution is finer along the main channel and slightly coarser on the shoals in order to accurately capture the salt intrusion and associated periodic strong stratification. The highest resolution is applied in the Chester River and Corsica River. The contrast in grid cell volume from the Bay main channel to the sub-tributary Corsica River is ~200:1 (Figure 2-5). This somewhat unconventional configuration is enabled by the implicit scheme in SCHISM, which allows us to almost arbitrarily refine regions of interest. Therefore, the cross-scale capability of SCHISM is clearly demonstrated with this set-up, allowing a seamless transition between larger- and smaller-scale processes, from main stem into small tributaries and into sub-tributaries.

Vertical discretization plays an equally important role in cross-scale problems. We utilize the LSC\(^2\) system (Zhang et al. 2015), which effectively reduces spurious diapycnal mixing between the deep channel and the adjacent shallow shoals (Figure 2-6). The slopes of the vertical coordinate planes are generally milder than the bottom slopes, effectively reducing the pressure gradient error (Haney, 1991). This is achieved by the use of the Vanishing Quasi-sigma (VQS) coordinate and shaved cells near bottom (cf. the enlarged view in Figure 2-6b). The vertical grid is also locally refined at mid-layers (around 1/3 depth from surface) to provide more resolution around the typical location of the observed pycnocline.
Figure 2-5: (a) Horizontal discretization, with quadrilaterals used in the main channels and near the head of the tributaries. The two enlarged views show the scale contrast: (b) between the upper Bay main channel and Chester River; (c) between Chester River and Corsica River. (d) Cumulative histogram of 3D prism volume distribution. The prism volume is the area of a 2D element times the vertical layer thickness.
Figure 2-6: Vertical discretization of a typical cross-channel transect: (a) the location of the transect in the grid (thick black line); (b) the vertical grid with an enlarged view in deeper depths.
With the aforementioned local refinements in both the horizontal and vertical dimensions, the model still runs stably at a time step of 120 seconds, courtesy of the implicit scheme. A constant drag coefficient with a typical value \(2.5 \times 10^{-3}\) is applied at the bottom boundary layer. Sensitivity tests using a roughness of 5 mm lead to similar results. The generic length scale model of \(k-k_l\) is used for turbulence closure (Umlauf and Burchard, 2003). Other turbulence closure schemes \((k-\epsilon\) and \(k-\omega\)) were also tested, and only minor differences were observed, which is consistent with Li et al. (2005)’s findings. The background diffusivity is set to \(10^6\) m\(^2\) s\(^{-1}\). Following Li et al. (2005), we tested the background diffusivity within the range of \(10^6\) to \(10^{-4}\) m\(^2\) s\(^{-1}\). Our results are consistent with theirs: the vertical salinity profile is not sensitive to background diffusivity when it is lower than \(10^{-5}\) m\(^2\) s\(^{-1}\), whereas a background diffusivity of \(10^{-4}\) m\(^2\) s\(^{-1}\) appears too large to adequately resolve the pycnocline. In simulating the heat flux from solar radiation, an albedo of 0.1 is used. Moreover, Jerlov type II water is specified, which is closer to the clearest ocean water than to muddy water (Paulson and Simpson, 1977) and seems to fit the UCB’s overall water condition.

The UCB model has been run on the high performance parallel computing system (SciClone Computing Complex) at the College of William & Mary. With 48 cores (Intel Xeon 5600-series processor, 3.2 GHz) on an HP ProLiant SL390s server, the simulation is 516 times faster than real time.

### 2.4 Model assessment

Standard statistics are used to assess the model errors against observation. These include: RMSE (Root Mean Square Error), bias, MAE (Mean Absolute error), CC (correlation coefficient). In addition, a target diagram (Jolliff et al., 2009) and a Taylor diagram (Taylor, 2001; Hofmann et al., 2008) are also used.

#### 2.4.1 Elevation
Both sub-tidal (Figure 2-7) and tidal (Figure 2-8) signals at tide gauges are analyzed. In general, the modeled free-surface elevation agrees very well with the observations. The correlation coefficients between the modeled and observed sub-tidal elevations are above 0.98 at four NOAA stations (Figure 2-7).

The amplitude and phase of the major constituents are well modeled as shown by the harmonic analysis (Figure 2-8); the largest error in M2 amplitude is only 4 cm, and the MAE of M2 phase is 13.9 minutes. The largest discrepancy between observation and model is found at Cambridge, which is likely due to the lack of grid resolution around that station because it is not an area of our interest. The phase errors at other stations are at most 13 minutes. Annapolis is near the semi-diurnal nodal area and its M2 amplitude is smaller than the other two main stem stations (Solomons and Tolchester), which is confirmed by the model results.
Figure 2-7: Subtidal surface elevation at two main stem stations (Annapolis and Tolchester) and two tributary stations (Cambridge and Baltimore). The CC and MAE are shown for each station. The storm event Hurricane Isabel (2003-09-18) is marked in the top panel.
2.4.2 Velocity profile

The velocity record at NOAA station cb1201 starts from March 2006, which is beyond the primary simulation period, so we use the alternative simulation period with NARR wind rather than hybrid wind (Section 3.2) for velocity validation. Figure 2-9 indicates that the velocity at the middle point of the UCB (cb1201) is adequately modeled at all layers with larger discrepancy near the surface. The CC’s from Layer 1 to Layer 9 (from surface to bottom) are: 0.73, 0.87, 0.88, 0.88, 0.87, 0.85, 0.81, 0.78, and 0.75. The observed surface velocity exhibits more variability than the model, likely due to the underestimation of gusts in the atmospheric model. The high model skill below the surface suggests that the density structure is well captured by the model.
Figure 2.9: Comparison of observed and modeled along-channel velocity profiles at cb1201.
2.4.3 Overall model skill in salinity and temperature

The overall salinity/temperature skill is based on an ensemble in space (at 9 CBP stations along the main channel) and time. The bias, RMSE, standard deviation, and CC between the model and observations are presented graphically in Figure 2-10 in the forms of target and Taylor diagrams. Each variable is normalized to the standard deviation of the corresponding observation so as to compare multiple variables on a single plot. On the target diagram, $x>0$ indicates an overestimation in the variability of the observations, while $x<0$ indicates an underestimation. More details on these diagrams are described by Hofmann et al. (2008), Jolliff et al. (2009), and Taylor et al. (2001). Besides our own model, the performance of the EPA regulatory model CH3D is provided as a state-of-the-art reference. It should be noted that the CH3D model is for the entire Chesapeake Bay, but the comparison shown here is confined to the UCB. A more direct comparison will be done between the 2 models once we complete a SCHISM simulation for the whole Bay. Nonetheless, Figure 2-10 suggests that the performance of our UCB model is quite good in terms of simulating the combined spatial and temporal variability of bottom salinity/temperature and surface salinity/temperature. In particular, the bottom salinity is well captured with a correlation of 0.99 to the observations. The two stratification indicators (the magnitude and the depth of the maximum vertical salinity gradient) have lower skill than those of the surface and bottom salinity. However, even with the lower skill associated with these variables, the model still performs better than the mean of the observations.
Figure 2-10: Target and Taylor diagrams illustrating the model skills of salinity and temperature at exact sampling times. Each variable is normalized by the standard deviation of the corresponding observed field. The SCHISM results are denoted by squares, and CH3D-ICM by circles. Different variables are denoted by different colors.

Table 2-1: The mean absolute error (MAE) and correlation coefficient (CC) of the modeled salinity/temperature at all sampling time and depth.

<table>
<thead>
<tr>
<th></th>
<th>at the exact sampling time</th>
<th>as the best match within a 6-hour window</th>
</tr>
</thead>
<tbody>
<tr>
<td>MAE of salinity (PSU)</td>
<td>1.08</td>
<td>0.86</td>
</tr>
<tr>
<td>CC of salinity</td>
<td>0.97</td>
<td>0.98</td>
</tr>
<tr>
<td>MAE of temperature (°C)</td>
<td>0.85</td>
<td>0.76</td>
</tr>
<tr>
<td>CC of temperature</td>
<td>0.99</td>
<td>0.99</td>
</tr>
</tbody>
</table>
2.4.4 Salinity

A transect along the main channel (location shown in Figure 2-4) provides an overview of the spatially varying yearly averaged (2004) salinity structure (Figure 2-11). It overlays the observations (CBP casts) on top of the model results; complete ‘disappearance’ of the observation points indicates a perfect model. The model generally captures the stratification structure and longitudinal salt transport well, with small over-estimation in the downstream and under-estimation upstream. The most discernable discrepancy is along the segment between CB3.1 and CB3.3C, where the largest vertical salinity gradient occurs. Within this region, the model generally under-estimates stratification.

Figure 2-11: Yearly (2004) averaged salinity on a longitudinal transect, with the observed values from CBP monthly/bi-monthly casts (filled circles) superimposed on the model results using the hybrid wind forcing (continuous color). Ideally, complete “disappearance” of the observation points indicates a perfect model. The locations of the transect and the stations are shown in Figure 2-4a.

For completeness, we present in supplementary materials the model-data comparisons for all observed salinity and temperature profiles (CTD casts) available to us. In these profiles, we include 1) model results at the sampling times; 2) best results within a 6-hour window to account for phase errors in the wind forcing. In general, the skills of these two sets of results
are close (Table 2-1; figures in supplementary materials) and only in rare cases are the shapes of the vertical profiles significantly improved by the time window (e.g. one snapshot on 2004-1-13 of all the 22 snapshots at CB3.3C; refer to supplementary materials). The uncertainties in the wind forcing play an important role in producing the large differences in these rare cases. For the few selected vertical profiles in the main text, we use the best match within a 6-hour window because they are mainly used in the discussion of wind mixing. Note that the vertical structure is more challenging to simulate than the bottom/surface salinity. We will discuss the highlights of these comparisons below.

Most of the vertical profiles are well reproduced by the model, with an overall MAE of 1.08 PSU, and CC of 0.97 (at exact sampling times). Most of the temporal and spatial gradients of salinity are successfully captured by the model. Unsurprisingly, the model error generally increases from downstream to upstream. The performance at the key station of CB3.3C, situated near a bifurcation point of channels, is quite satisfactory. This station is also located in a zone where some interesting processes occur, for example the three-layered circulation in the adjacent Baltimore Harbor (Section 2.5.3). Larger errors are seen at stations upstream of CB3.3C, as the salinity intrusion gradually weakens into the freshwater zone.

The model also generally captures the mixed-layer depth, which has been shown as a key parameter for hypoxia, water quality, and habitat (Irby et al., 2016). Occasionally, strong mixing due to wind can be seen in this layer. This phenomenon is common in winter and early spring during storms (Figure 2-12a; also see sub-plots 2003-12-17 ~ 2004-3-17 in Fig. A-4, supplementary material). The longitudinal transect in Figure 2-12b shows one such mixing event that has led to large vertical diffusivity in the surface layer. However, the model did not capture some of the more complex multi-layered profiles (e.g., 2004-4-27 and 2004-9-21 at CB4.1C, Fig. A-3, supplementary material). Furthermore, a few instances of extremely sharp pycnoclines (e.g., 2004-5-25 at CB4.1C, Fig. A-3) were not well resolved. This is likely due to
the inadequacy in wind forcing rather than grid resolution, because fairly sharp pycnoclines have been captured by the model at other times (e.g., 2004-1-13 at CB3.3C, Figure 2-12a; 2004-9-21 at CB3.3C, supplementary materials). Further efforts are needed to construct more accurate wind forcing from atmospheric model results and observation.

Figure 2-12: (a) A vertical salinity profile at CB3.3C showing a typical “staircase” pattern, with mixed layers at surface and bottom, and an abrupt transition at mid-depth. (b) Modeled log-transformed vertical eddy diffusivity (continuous colors) overlaid with salinity (PSU) contours (white lines) along a longitudinal transect; the location of CB3.3C is highlighted.

Accurate simulation of stratification/destratification is challenging for estuarine models in general. Under normal conditions, the model adequately reproduces the periodical stratification/destratification (Figure 2-13). Under extreme events such as the Hurricane Isabel, the model also captures the wind-induced destratification and the subsequent recovery to a stratified state. Before the storm event, there was a significant amount of stratification in the water column, with the bottom-surface difference ($\Delta z_S$) up to 11 PSU (2003-9-16, Figure 2-14a). This value dropped to below 1 PSU immediately after Hurricane Isabel (2003-9-23, Figure 2-14b) and returned to the pre-storm condition by the next sampling date (2003-10-7, Figure 2-14c). The model qualitatively reproduced these three phases, capturing at least two major mixing events during the course of the hurricane (Figure 2-15a and b). The first one is upon Hurricane Isabel’s arrival on 2003-9-18 (Day 260 in Figure 2-15), which is almost certainly due to wind mixing. The second one is on 2003-9-23 (Day 265 in Figure 2-15), and
is confirmed by the CBP observation. However, an under-estimation of storm induced mixing is evident as shown in Figure 2-14b and Figure 2-15b. Again, the under-estimation of wind intensity in the forcing may be responsible for this discrepancy, but other potential causes include: 1) errors from the salinity boundary condition, which varies linearly between two sampling dates thus does not adequately resolve storm events; 2) errors from parameterizing non-hydrostatic processes such as Langmuir turbulence in a hydrostatic model.
Figure 2-13: Time series of bottom-surface salinity difference ($\Delta_z S$) at: (a) main channel stations and; (b) side channel stations.
Figure 2-14: The observed and modeled vertical salinity profiles at CB3.3C (a) before, (b) during and (c) after Hurricane Isabel.

Figure 2-15: The observed and modeled (a) surface/bottom salinity and (b) bottom-surface salinity difference ($\Delta_s$) at CB3.3C, with the arrival of Hurricane Isabel indicated.
2.4.5 Temperature

The modeled water temperature generally has high skill, with an averaged MAE of 0.85 °C and CC of 0.99 based on the results at the sampling times. A distinctive feature of temperature is that the vertical gradient changes signs in spring and fall, which is adequately reproduced by the heat exchange model inside SCHISM (Figure 2-16). The vertical temperature profiles at all stations are presented in supplementary material (Part B) in the same fashion as the salinity profiles. Some complex thermal structures closely follow those of salinity (Fig. B-3, Sept. 21), suggesting that temperature can be mostly regarded as a tracer in this salinity-dominated environment.

![Figure 2-16](image)

Figure 2-16: Observed and modeled (a) temperature and (b) bottom-surface temperature difference ($\Delta T$) at CB3.3C.

2.5 Results and discussion

2.5.1 Transport scheme

Sensitivity tests were conducted to compare the efficiency and accuracy of the new transport solver with the old explicit TVD solver. The UCB grid has a typical prism volume of $10^5$ m$^3$ (with horizontal length of 330 m and vertical layer thickness of 0.9 m) in the main stem, and $5\times10^2$ m$^3$ (horizontal length of 60 m and vertical layer thickness of 0.14 m) in the refined Corsica River, which translates to a volume contrast of 200:1. Compared to the model
simulation with the explicit transport solver, the new implicit solver reduces 28% of the total computational cost (i.e., a speedup of 1.4). This efficiency benchmark is compared with those conducted in other systems (Table 2-2). In general, the speedup is positively correlated with 1) scale contrast, and 2) bathymetry slope. Here, maximum bottom slope serves as a surrogate for largest vertical velocity. Note that only two tracers (salinity and temperature) are involved in these tests, so larger speedup is expected when more tracers are involved, as in a typical water quality simulation.

Table 2-2: The efficiency of the new solver in various applications.

<table>
<thead>
<tr>
<th>References</th>
<th>Upper Chesapeake Bay</th>
<th>San Francisco Bay (Ateljevic et al., 2015)</th>
<th>Black Sea (Zhang et al., 2016)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Total elements</td>
<td>26,027</td>
<td>153,993</td>
<td>177,758</td>
</tr>
<tr>
<td>Total nodes</td>
<td>16,374</td>
<td>164,016</td>
<td>104,211</td>
</tr>
<tr>
<td>Average vertical layers</td>
<td>23.5</td>
<td>10.6</td>
<td>34.8</td>
</tr>
<tr>
<td>Typical prism volume in coarse areas (m$^3$)</td>
<td>$10^5$</td>
<td>$10^6$</td>
<td>$3\times10^8$</td>
</tr>
<tr>
<td>Typical prism volume in refined areas (m$^3$)</td>
<td>$5\times10^2$</td>
<td>10</td>
<td>$10^5$</td>
</tr>
<tr>
<td>Prism volume contrast</td>
<td>($2\times10^2$):1</td>
<td>$10^4$:1</td>
<td>($3\times10^3$):1</td>
</tr>
<tr>
<td>Maximum bottom slope</td>
<td>0.06</td>
<td>0.7</td>
<td>0.5</td>
</tr>
<tr>
<td>Speedup</td>
<td>1.4</td>
<td>1.5</td>
<td>2.6</td>
</tr>
</tbody>
</table>

The accuracy of the implicit solver is evidenced by its superior skill in capturing the stratification. The strong stratification in the Upper Bay is challenging and is usually underestimated by models (Irby et al., 2016). For the yearly (2004) averaged salinity along the main channel transect, the stratification predicted by the implicit solver is consistently larger than that predicted by the explicit solver (Figure 2-17a), reducing the RMSE from 1.49 to 0.49 PSU. Moreover, the new solver often produces a sharper pycnocline (Figure 2-17b). This is consistent with the numerical benchmarks discussed in Section 2.2.
Figure 2-17: Comparisons between the new transport solver and the old transport solver (explicit TVD): (a) yearly (2004) averaged bottom-surface salinity difference along a longitudinal transect; (b) a snapshot of the vertical salinity profile at CB3.3C. The locations of the transect and the stations are shown in Figure 2-4a.

2.5.2 Wind forcing

Wind forcing plays a critical role in producing the mixed layer as shown in Figure 2-12. We illustrate the importance of wind forcing by comparing two sets of results generated by the hybrid wind and the original NARR wind in Figure 2-18. Under normal conditions, the difference in wind forcing is only appreciable in the water column less than 10 meters below surface. Therefore, the shallow shoals are more sensitive to wind forcing than the deeper center channel (Figure 2-18a and b). Under storm events, however, the entire water column is mixed even in the deep channel (Figure 2-18c). In general, the hybrid wind has more high-frequency fluctuations than NARR wind (Figure 2-18d and e), and the magnitude of the hybrid wind is larger than NARR wind during Hurricane Isabel (Figure 2-18e). The hybrid wind produced better results in all cases than the original NARR wind. However, the stratification is still over-predicted during storm conditions, probably because the hybrid wind still under-estimates wind intensity, or due to other causes mentioned at the end of Section 2.4.4.
Figure 2-18: The effect of wind forcing on the modeled salinity profiles: (a) main channel; (b) side channel; (c) main channel during hurricane Isabel. The wind forcing for (a) and (b) is shown in (d). The wind forcing for (c) is shown in (e).
2.5.3 Cross-scale capability

While the previous discussions focus on the main stem of UCB, we now turn to a few tributaries to demonstrate the model’s cross-scale capability.

*Baltimore Harbor*

Baltimore Harbor is located on the western shore of the Chesapeake Bay, and connects to the main bay via a dredged channel about 30 m deep (Figure 2-4). The most distinctive feature of the Baltimore Harbor is a vertically three-layered sub-tidal circulation, which is controlled by a unique salinity distribution in this area (Chao et al., 1996; Schubel and Pritchard, 1986; Stroup et al., 1961). The spring freshet of Susquehanna River is the main driver of the salinity distribution and circulation patterns in the Baltimore Harbor. Some features that further promote the three-layered circulation include: 1) small fresh water inputs inside the Harbor; 2) a deep and straight artificial channel from the Bay main stem to the Harbor.

Our results are in close agreement with the schematic depictions and observations in early studies (e.g., Figure 2-9 in Schubel and Pritchard, 1986). In the monthly averaged model results in 2004, the three-layered pattern is most pronounced in April (Figure 2-19a), when the Bay main stem is fresher than the Harbor in surface layers due to the spring freshet. As the fresh water discharge from the Susquehanna River continues to increase through May, the vertical and longitudinal salinity gradient decreases. As a result, the modeled three-layered circulation pattern weakens: the surface inflow and mid-layer outflow are still present, but the magnitude of the bottom flow is reduced near the mouth (Figure 2-19b). As fresh water input decreases in summer, the Bay becomes saltier than the Harbor. The monthly averaged circulation in July inside the Harbor resembles a classic estuarine circulation with surface outflow and bottom inflow (Figure 2-19c). Therefore, the accurately simulated salinity in the bay main stem is important in capturing the circulation inside the Harbor.
Figure 2-19: Simulated monthly average salinity distribution and circulation patterns inside the Baltimore Harbor (0-15 km) and the adjacent bay (15-17 km) in 2004. The location of the transect is shown in Figure 2-4a.
Chester River

Chester River is characterized by its shallow (8.4 m) but wide mouth and a deep (up to 16 m) but narrow main channel. Narrower minor channels are also found in sub-tributaries like the Corsica River. We are making efforts to understand the severe water quality issue in this impaired system and to identify optimal management strategies for nutrient reduction. Since the advection and mixing processes are of fundamental importance for biogeochemical processes, accurately simulating hydrodynamic variables such as salinity and temperature is a pre-requisite for successful water quality simulations.

The Chester River tributary and its sub-tributary, the Corsica River, are locally refined in the model grid (Figure 2-5a) to provide more accurate transport field. In this region, 2838 elements were added during the refinement, increasing the prism volume contrast from 5:1 to 200:1. This would have significantly slowed down the explicit solver; but with the new solver (running on the same type and number of CPUs) the computational cost only increased by 17.0%, which is only slightly greater than the increase in the number of elements (13.3%). In other words, the model exhibits good weak parallel scaling.

The largest stratification is found at station ET4.2 (location shown in Figure 2-4a), where the bottom-surface salinity difference fluctuates between 2 PSU to 8 PSU over a water depth of 13.4 m. This pattern is largely determined by the fluctuations of the salt intrusion from the main stem, as the freshwater inputs from the adjacent watershed are mostly small. The model captures this trend well, although the maximum stratification is under-estimated (Figure 2-20). The discrepancy is likely due to the uncertainty in the point and non-point sources of freshwater inputs, which have larger impact on smaller tributaries like Chester River than on the main stem.
Figure 2-20: Observed and modeled (a) bottom/surface salinity and (b) bottom-surface salinity difference (\(\Delta s\)) at the Chester River station ET4.2.

The sub-tributary Corsica River (Figure 2-5b) is of particular interest because of its very poor water quality mostly due to extensive phytoplankton blooms. The transport process must be adequately simulated for the water quality studies. The 15-minute continuous salinity observations from three CMON stations (XHH4916, XHH4931, and XHH3851) allow rigorous tests on model performance in this shallow region. However, the available data start from 2005 for XHH3851 and 2006 for the other two stations. Therefore, we select the results from our 2003~2010 UCB simulation with NARR wind for model data comparison. As in the UCB main stem, structured quadrilateral elements are used in the main channel, and triangular elements are used elsewhere to fit the complex geometry in the shoals (Figure 2-5b). Previously, the base model without local refinements in the Corsica River generally underestimates salinity by 2 PSU. After the modest refinements described earlier, the model successfully captures the salt intrusion (Figure 2-21).

The local refinement capability of SCHISM as demonstrated by this example is significant for management. As increasing attention is being paid to the highly productive shallows, it’s imperative that we understand the connections between remote forcings and local response, as the shallows are strongly influenced by both local and remote forcings.
Figure 2-21: Comparison of salinity between continuous monitoring data and model results at three Corsica River stations.

2.6 Conclusions

We have successfully incorporated a new implicit transport solver with two TVD limiters (in space and time) into a 3D baroclinic model on unstructured grids (SCHISM), and applied it to the complex physical processes found in the Upper Chesapeake Bay. Together with other new model capabilities we have recently developed (hybrid tri-quad elements, LSC$^2$ vertical grid), we showed that the model is both accurate and efficient for this system. In particular, the surface elevation is well simulated. The velocity, salinity and temperature and their vertical structures are also well captured by the model. The model also successfully reproduces the typical multi-layer structures as observed in the Baltimore Harbor. The new model is very flexible in its horizontal and vertical grids, and thus can be effectively applied to study the cross-scale problems facing the environmental managers in this region. We demonstrated this by extending high grid resolution into a tributary (Chester River) and its sub-tributary (Corsica River).
On a wider perspective, the techniques utilized in the UCB model work equally well in a wide range of systems (Zhang et al., 2016a). The implicit TVD solver significantly reduces computational cost, which is invaluable not only for SCHISM but also for other unstructured models that utilize highly variable grid resolution. Moreover, the proper representation of the above-mentioned physical processes is important for water quality and biological studies in UCB and elsewhere. In this vein, the techniques presented in this paper represent a powerful tool in our understanding of the impact of both local and remote forcings on estuarine systems, which can ultimately lead to a holistic management strategy.
3 Medium domain: Assessment of a 3D unstructured-grid model for the Chesapeake Bay and adjacent shelf and importance of bathymetry

(Adapted from Ye et al. Ocean Modeling (in revision))

Abstract

We extend the 3D unstructured-grid model previously developed for the Upper Chesapeake Bay to cover the entire Bay and its adjacent shelf, and assess its skill associated with the 3D baroclinic processes responsible for generating saltwater intrusion and the coastal plume. Recently developed techniques, including a flexible vertical grid system and a 2nd-order, monotone and implicit transport solver are critical in successfully capturing the baroclinic processes. Most importantly, good accuracy is achieved through an accurate representation of the underlying bathymetry, without any smoothing. The model in general exhibits a good skill for all hydrodynamic variables: the averaged root-mean-square errors (RMSE’s) in the Bay are 9 cm for sub-tidal elevation, 17 cm/s for 3D velocity, 1.5 PSU and 1.9 PSU for surface and bottom salinity respectively, 1.1 °C and 1.6 °C for surface and bottom temperature respectively. On the shelf, the average RMSE is 18 cm/s for surface velocity, and 1.4 °C for surface temperature. We highlight, through results from sensitivity tests, the central role played by bathymetry in this estuarine system and the detrimental effects, from a common class of bathymetry smoothers, on volumetric and tracer fluxes as well as key processes such as the channel-shoal contrast in the estuary and plume propagation in the coast.

Keywords: bathymetry; cross-scale; SCHISM; estuarine circulation; Chesapeake Bay, USA
3.1 Introduction

Previously we have developed several new numerical techniques and incorporated them into a 3D unstructured-grid (UG) model (SCHISM, i.e., “Semi-implicit Cross-scale Hydroscience Integrated System Model”; Zhang et al., 2016a) and applied it to the Upper Chesapeake Bay (Ye et al., 2016). With the new transport solver developed in Chapter 2, the model was shown to be able to accurately simulate saltwater intrusion and density stratification in the system, and can be readily extended into small tributaries and sub-tributaries. We continue previous work by extending the model to cover the entire Bay and a portion of the Mid Atlantic Bight (MAB) shelf. The rationale for including the shelf is to incorporate shelf processes as much as possible, because these and Bay processes are intertwined (Xu et al., 2011). This approach also allows us to systematically examine the effects of ocean boundary conditions (B.C.).

Several other models based on SGs or UGs have been applied to the Bay (Li et al., 2005; Cerco et al., 2010; Lanerolle et al., 2011; Hong and Shen, 2012; Testa et al., 2014; Feng et al., 2015; Jiang and Xia, 2016) and an inter-comparison of some of these models can be found in Irby et al. (2016). Major departures of the current model from previous models are: (1) use of high-resolution hybrid triangular-quadrangular UG; (2) use of a novel hybrid vertical grid in order to seamlessly traverse contrasting spatial scales from sub-tributaries to shelf; (3) an accurate representation of the original bathymetry through the combination of (1) and (2) and courtesy of the implicit scheme that allows large time steps (in this case 2.5 minutes) in conjunction with high resolution. Consequences from these choices are discussed in this chapter, and the detrimental effects of bathymetry smoothing on volumetric/tracer fluxes and other important variables will be highlighted.

In the following sections, we first describe the observational datasets used in this chapter (Section 3.3.1), and then provide a description of the model set-up (Section 3.3.2 and 3.3.3). The model skill is then assessed in the Section 3.4. We then present a sensitivity study on the
importance of model representation of the underlying bathymetry (Section 3.5). The influence of the ocean boundary condition is briefly discussed in Section 3.6 as a precursor to Chapter 4. Section 3.7 summarizes the chapter.

3.2 Observations used for model evaluation

The Chesapeake Bay and adjacent shelf is a well-instrumented system with extensive in-situ and remote sensing observational assets. EPA’s Chesapeake Bay Program Office (CBPO) maintains a network of stations and regularly conducts synoptic surveys throughout the Bay (usually bi-weekly in summer or monthly in winter); the measured variables include both physical and biogeochemical variables. The modeled salinity and temperature profiles are compared to CBPO observations.

NOAA maintains over 40 tide gauges in and around the Bay and adjacent shelf (https://tidesandcurrents.noaa.gov/tide_predictions.html, last accessed in April 2017). In addition, PORTS (https://tidesandcurrents.noaa.gov/ports.html, last accessed in April 2017) also maintains ADCPs at a few stations in the Bay during some recent years; the velocity data are used to validate our modeled current profiles.

To evaluate model skill on the shelf, we use a daily, global 1 km operational Sea Surface Temperature (SST) product based on satellite data called G1SST (https://podaac.jpl.nasa.gov/dataset/JPL_OUROCEAN-L4UHfnd-GLOB-G1SST, last accessed in April 2017), where various SST datasets at different spatial resolutions are combined with a multi-scale two-dimensional variational (MS-2DVAR) blending algorithm (Chao et al. 2009). Although we use G1SST as “observation” in this paper, it actually represents an optimal estimate of skin SST, and the modeled SST is a bulk estimate at the sea surface. Surface current observations are taken from the Coastal Observing Research and Development Center (http://cordc.ucsd.edu/projects/mapping/, last accessed in March 2017) that manages
and distributes ocean surface currents in near-real-time measured by a distributed network of shore-based HF radar systems.

We focus on the recent period of 2011-2014 to maximize data availability. In addition, the long-term observational datasets described above are supplemented by a campaign survey in 1996-1997 that occurred during one of the wettest periods in recent history. In Section 3.4.6 we present the dataset collected during this survey and use it to assess model results in the plume region. All observational assets used in this chapter are summarized in Figure 3-1.
3.3 Model configuration

The model SCHISM (Zhang et al., 2016a; Ye et al., 2016) is a derivative product of SELFE v3.1dc (Zhang and Baptista, 2008), but freely distributed using an Apache v2 license. It is an open-source community-supported modeling system, based on mixed triangular-quadrangular...
unstructured grids in the horizontal and a very flexible coordinate system in the vertical (Zhang et al., 2015), designed for the effective simulation of 3D baroclinic circulation across creek-to-ocean scales (Zhang et al., 2016a; Yu et al. 2017). The model employs a semi-implicit finite-element/finite-volume method, together with an Eulerian-Lagrangian method for momentum advection, to solve the Navier-Stokes equations in its hydrostatic form. As a result, numerical stability is greatly enhanced and the errors from the “mode splitting” method are avoided; in fact, the only stability constraints are related to the explicit treatment of the horizontal viscosity and baroclinic pressure gradient, which are much milder than the stringent Courant-Friedrichs-Lewy (CFL) condition. The implicit scheme used in SCHISM often allows the selective use of “hyper resolution” (on the order of a few meters) with little penalty on the time step. More information about the model and its application cases around the world can be found at www.schism.wiki (last accessed in April 2017).

Some recent model developments include: (1) addition of share-memory protocol via openMP on top of existing domain decomposition (via Message Passing Interface) to improve strong scaling on large-core count high-performance systems; (2) optional matrix solvers via PETSc (https://www.mcs.anl.gov/petsc/, last access in March 2017); (3) addition of a vegetation model and a marsh migration model. The version of SCHISM used in this paper is the publicly released tag version v5.3.1, freely downloadable at www.schism.wiki (last accessed in Jan 2017). We use this public version and upload some key files as supplementary materials to promote reproducibility of the results.

3.3.1 Digital Elevation Model (DEM) and bathymetry

There are multiple publicly available DEMs for the Chesapeake Bay and adjacent shelf region. The DEM used here is primarily based on the topo-bathymetric information from USGS (https://topotools.cr.usgs.gov/coned/chesapeake_bay.php; last accessed in Feb. 2017),
supplemented by the latest navigation charts (especially around Baltimore harbor area), and coastal relief model (https://www.ngdc.noaa.gov/mgg/coastal/crm.html, last accessed in Jan 2017) for the coastal and shelf region. Bathymetric changes due to regular dredging by USACE are not explicitly accounted for, but are treated as part of the model uncertainties. Since our grid resolution is much coarser than the original USGS DEM’s 1 m resolution, the DEM was subsampled to 45 m to reduce its size. In order to easily incorporate new DEMs in small tributaries and sub-tributaries in the future, we have triangulated the original raster files to generate an UG DEM (Figure 3-2), which can be found in supplementary materials (doi:10.21220/V5HK5S).
The bathymetry in the Bay has several key features. There is a main shipping channel (~15-40 m depth) that cuts through the otherwise shallow estuary and extends from the Atlantic to Baltimore harbor. The channel is regularly dredged and maintained to make it navigable by megaships. Still, the channel is “interrupted” by shallow shoals at places (e.g. Figure 3-2c). It also branches off into multi-channel configuration at other places (Figure 3-2ad). As will be shown in Section 3.5.1, the channel-side slopes often exceed 1:2. The channel width varies from ~5 km near the entrance to ~400 m near Baltimore harbor (Figure 3-2a). The channel also
turns abruptly at places (Figure 3-2acd), which is conducive to secondary circulation (Pein et al. 2014). Adequate bathymetric resolution is required to capture those channel constrictions (Figure 3-2acd), which have important implications for hydrodynamic processes in the Bay.

Figure 3-3: SMS map for (a) lower Bay; (b) upper Bay; (c) typical channel representation in SCHISM, with 2 nodes dispensed to represent each channel edge (one at the top and the other at the foot of the edge). In practice, more nodes may be inserted on the edge and the bottom portions.

3.3.2 Grid generation

Our computational grid covers the entire Bay from Cape Henry to the Conowingo Dam in the Susquehanna River. The opening to the Delaware Bay through the Chesapeake & Delaware canal is closed in the grid since the dynamics there are generally believed to be insignificant for main Bay processes; preliminary test results support this hypothesis, though more carefully controlled tests are needed in the future. The grid also covers a portion of the MAB, up to Lewes, DE in the north and Beaufort Inlet, NC in the south, and out to the 3 km isobath (slightly
beyond the shelf break) offshore. The inclusion of the shelf allows us to avoid significant influence from the boundary condition (B.C.) imposed there and to systematically evaluate the influence of B.C.’s imposed at the open ocean (Section 3.6). Since the domain includes part of the Gulf Stream, we rely on the B.C. from the data-assimilated HYCOM (hycom.org, last accessed in Jan 2017) to bring its signal into the domain.

Due to its semi-implicit numerical algorithm and specific horizontal and vertical grid systems, SCHISM often incurs no time stepping penalty on local resolution, so relative to prior modeling efforts in this domain, we can faithfully represent key features (channels, shelf breaks, jetties, etc.). For example, finer resolution in the shipping channel (as compared to the shoals) is usually needed to accurately capture the saltwater intrusion process, but refining deeper areas rather than shallow would have been contrary to the requirements arising from the CFL condition for explicit models. Additionally, the SCHISM formulation is very tolerant of skew elements, which helps us align the mesh to contours and breaks. Figure 3-3 is a map showing contours that are enforced as part of our grid generation process (excerpted from the “map” file from SMS software (aquaveo.com, last accessed in Jan 2017)). The channel edges (based on the highest gradient of the isobaths) and shelf break are captured by carefully aligning element edges to these features. Often the channel profile is represented by at least 4 nodes, with 2 nodes dispensed to represent each channel edge (one at the top and the other at the foot of the edge; Figure 3-3c). Meshing in this way causes the feature-aligned arcs to be close to each other on steep channel slopes (Figure 3-3ab), resulting in skew elements, but the implicit model can deal with elements with the skewness (defined as the ratio between the maximum side length and the equivalent diameter of an element) exceeding 20. Once the important features to be aligned have been digitized, the hybrid triangular-quad grid is generated. The grid resolution is primarily controlled by the arc resolution. The final computational grid has 28,137 nodes, 35,756 triangles and 8,833 quads (Figure 3-4).
Figure 3-4: Horizontal grid with zooms. Average resolution in each region is also provided.
Mesh bottom elevations for the present model are populated by a linear interpolation from the DEM. Such a method is consistent with the linear shape function used in the finite-element framework in SCHISM. The use of shaved cells near the bottom ensures a smooth and continuous representation of the bottom. Although the combined procedure is 2nd-order in its representation of bottom, if the mesh is not sufficiently resolved it can lead to systematic loss of volume in convex channels – a small amount of such loss can be seen in Figure 3-3c as the region between the linear bottom and the “true” bed. Importantly, the mesh is not smoothed. We later perform sensitivity studies on bathymetry smoothing, which is often used with terrain-following coordinate models. The implication of the smoothing procedure will be discussed in Section 3.5.

As in Ye et al. (2016) the model uses the new flexible vertical grid system LSC$^2$ (Localized Sigma Coordinates with Shaved Cells) developed by Zhang et al. (2015), which is a generalization of the Vanishing Quasi-Sigma Coordinates of Dukhovskoy et al. (2009). Shaved cells are added near the bottom to ensure a smooth (piece-wise linear), staircase-free bottom representation. The latter has been demonstrated to be essential for successfully capturing the bottom controlled processes such as saltwater intrusion (Ye et al. 2016) and dense water overflow along steep slopes (Zhang et al., 2016ab; Stanev et al., 2017). The number of levels in the final vertical grid varies from 16 (at 8 m depth) to 67 (at 4000 m depth), and 24.6 on average. Figure 3-5 shows typical configurations of the vertical grid in and outside the Bay. High resolution is applied near the surface and bottom, but the mid depths inside the Bay are also adequately resolved in order to capture the sharp pycnocline there. In generating the vertical grid, we have used two master grids (see Zhang et al., 2015 for more details on master grids), designed for the Bay and shelf portions of the domain respectively and “stitched” together at a common depth near the Bay entrance (Figure 3-5bc). The flexibility afforded by LSC$^2$ allows us to apply resolution almost at will (as each horizontal node can have its own
vertical grid), although abrupt transitions in the number of levels should be avoided in practice as they may lead to excessive momentum dissipation.
Figure 3-5: Vertical grid. (a) Transect location from the upper Bay to the shelf break; (b) master grid used for the Bay portion; (c) master grid used for the shelf portion; (d) 3D grid as seen along the transect shown in (a); (e) zoom-in in a stretch of the Bay. Note the shaved cells near the bottom used to ensure a smooth representation of the bottom.
3.3.3 Forcing

The primary simulation period of 2011-2014 includes some typical variability of the hydrological flow regime: a wet year in 2011, a dry year in 2012 (with a below-average spring freshet), average years in 2013 and 2014, and two storms (Hurricane Irene in Aug. 2011 and Hurricane Sandy in Oct 2012) (Figure 3-6a). In addition, we’ll also present an extreme case as occurred in the strong El Nino year of 1996 with large freshets (Figure 3-6b). To more accurately simulate the salinity in the Bay we opted to use the watershed loadings calculated from CBP’s watershed model (Shenk and Linker, 2013) for years 2011-2014; we found that the results from this approach were slightly more accurate than those using the river flows at the seven major tributaries (Susquehanna, Patuxent, Potomac, Rappahannock, Pamunkey, Mattaponi, and James) as measured by USGS gauges, suggesting influence from smaller tributaries may not always be negligible. The total amount of fresh water flows into the Bay from the two approaches are generally similar but sometimes differ significantly (Figure 3-6a), especially during autumn and winter, when the total flow from the watershed model is often larger. The watershed model loadings include the inflows from smaller tributaries and sub-tributaries, the effects of which are locally very important.
A hybrid wind dataset blending North American Regional Reanalysis (NARR) and NDBC buoy observations is generated using the simple method proposed by Lanerolle et al. (2011). Compared to Lanerolle et al. (2011)’s early work, more NDBC buoys are available in the primary simulation period and are incorporated into the hybrid wind product, providing a more extensive coverage inside the Bay (see supplementary materials). Compared to the pure NARR wind, the hybrid wind possesses more spatial/temporal variability and gusts. As shown in Ye et al. (2016), the use of the hybrid product leads to a more realistic wind-induced mixing. Other atmospheric forcing applied at the surface is taken from NARR, including: atmospheric pressure (important during storms), downward short-wave and long-wave radiation fluxes, air temperature, specific humidity, and precipitation. The effect of direct precipitation is also included but is found to be mostly negligible. The atmospheric forcing is then used to calculate...
the momentum and heat exchanges between the air and water via the bulk aerodynamic model of Zeng et al. (1998).

At the ocean boundary, the imposed elevation is interpolated from two tide gauges at Lewes, DE and Beaufort, NC, using the inverse distance interpolation method. The difference in phase/amplitude between each boundary point and the two tide gauges are also considered, based on the result of a 2D barotropic SCHISM model on a larger grid that encompasses the entire east coast of US. This approach ensures that both tidal and sub-tidal signals are incorporated in the model. The horizontal velocity B.C. is a linear superimposition of a tidal component generated by the large-domain 2D barotropic SCHISM model and a non-tidal component from the daily outputs from HYCOM. The salinity B.C. is interpolated from the monthly climatology of World Ocean Atlas 2001 (http://www.nodc.noaa.gov/OC5/WOA01/pr_woa01.html, last accessed in Jan 2017). The temperature B.C., on the other hand, is interpolated from HYCOM to better account for inter-annual variability for this variable. In addition, the simulated salinity and temperature are also relaxed towards climatology/HYCOM respectively in a region ~30 km near the ocean boundary, with a maximum temporal relaxation scale of 0.5 days, in order to prevent long-term drift. The relaxation constant decreases linearly from its maximum value at the ocean boundary to 0 at ~30 km from the boundary.

Initially the water is at rest. The initial 3D salinity/temperature field inside the Bay is interpolated from the observations at CBP Water Quality Monitoring stations along the main shipping channel (Figure 3-1): salinity and temperature are first interpolated along the longitudinal transect, and then laterally extrapolated in the cross-channel direction at each depth. The initial temperature and salinity on the shelf are interpolated from HYCOM/climatology respectively.
The model uses a non-split time step of 150 s, the implicitness factor of 0.6, and turbulence closure of k-kl (Umlauf and Burchard, 2003). A uniform drag coefficient of 0.0025 is used for simplicity. The MB-LI scheme, stabilized by a Shapiro filter is used to treat the momentum advection (Zhang et al., 2016a). No explicit horizontal viscosity or diffusivity is applied in the model; note that the higher-order TVD^2 transport solver is monotone by design (Ye et al., 2016). Since the mean residence time in the modeled region is about 3 months estimated from an average flow year (Hong and Shen, 2012) and at most 6 months in the dry period (Du and Shen, 2016), the model is initialized 6 months before the periods of interest. On 48 Intel XEON cores of the SciClone cluster at College of William & Mary, the model runs 405 times faster than real time.

3.4 Model assessment

Consistent with Ye et al. (2016), we use standard statistics to assess model errors against observation, including: RMSE (Root Mean Square Error), MAE (Mean Absolute Error), bias and CC (correlation coefficient). The simulated elevation is compared to observation at 8 NOAA stations from the coastal region to the inside of the Bay. The simulated velocity is compared to the multi-layer ADCP measurements at 3 locations from the Bay mouth to the upper Bay. The overall salinity and temperature skill is based on an ensemble in space (at 39 CBP Water Quality Monitoring stations in the Bay; Figure 3-1). The bias and RMSE between the model and observations are summarized in the form of target diagram (Figure 3-7). Each variable is normalized to the standard deviation of the corresponding observation type so as to compare multiple variables on a single plot. On the target diagram, $x>0$ indicates an over-estimation in the variability of the observations, while $x<0$ indicates an under-estimation. More details on these diagrams are described by Hofmann et al. (2008) and Jolliff et al. (2009).
The presentation of individual results will be focused more on salinity given its importance for density stratification. Most stations shown are in the main stem of the Bay; model assessment in the tributaries has been discussed elsewhere (Ye et al. 2016).

![Target diagram for salinity and temperature model skill.](image)

**Figure 3-7:** Target diagram for salinity and temperature model skill.

### 3.4.1 Elevation

Both sub-tidal and tidal signals at seven NOAA tide gauges along the Bay main stem are compared to the SCHISM output. In general, the modeled free-surface elevation agrees well with the observations. The correlation coefficients between the modeled and observed sub-tidal elevations are above 0.78, and the RMSE’s are below 12 cm at all stations. For the subtidal elevation, the averaged RMSE and CC over all stations are 9 cm and 0.84 respectively. For the total elevation (including both tidal components and sub-tidal components), the averaged RMSE and CC over all stations are 11 cm and 0.90 respectively. The hurricane induced set-ups are also captured by the model (e.g., Hurricane Irene in Figure 3-8).
Figure 3-8. Time series of total (tidal plus sub-tidal) elevation, showing a typical period including normal conditions and a storm condition at one station (CBBT) near the Bay mouth.

The amplitudes and phases of the major constituents are well modeled as shown by the harmonic analysis (Figure 3-9); the largest error for the M2 amplitude is only 1.8 cm, and 3.9 degrees for the M2 phase. The model tends to over-estimate the amplitudes except at Annapolis, where the largest error happens to occur (Figure 3-9). Annapolis is near the semi-diurnal nodal area and its M2 amplitude is smaller than the other two main stem stations (Solomons and Tolchester), which is confirmed by the model results. Other constituents are also accurately simulated. The rapid decrease of the M2 amplitude from the lower to upper Bay indicates that the Bay is a highly dissipative system as discussed by Zhong et al. (2008).

Figure 3-9. Tidal harmonics for 4 major constituents from 2011-2014.
3.4.2 Velocity profile

Three NOAA/PORTS ADCPs in the lower, mid and upper Bay (Figure 3-1) were operational in parts of 2012-2014, and the data are used to assess the vertical structure of the along-channel velocity. The barotropic velocities are primarily driven by river flows, tides and winds. The good agreement in the simulated elevations translates into good skill for the barotropic velocity (Figure 3-10). The averaged RMSE in 2012-2014 for all stations is 16 cm/s. Significant baroclinic effects are found at all stations due to persistent density stratification, and the model captures the baroclinic velocity structure well (Figure 3-11). At station cb0102 (Bay mouth), larger discrepancies are found near the surface, likely due to an under-estimation of gusts in the atmospheric model or inaccuracy in the turbulence closure model. At the two upper Bay stations, larger discrepancies are found near bottom, likely due to the uncertainties in bathymetry (the channel is regularly dredged in this region). Overall, the averaged CC’s at the three stations are 0.89, 0.88, and 0.92 respectively, and the averaged RMSE’s (which include some small phase errors) are 21, 15, and 13 cm/s respectively, or 17 cm/s overall; therefore, the main error source is of barotropic origin (more precisely, the small phase error). The good agreement for the baroclinic velocity suggests that the density structure is also well simulated.
Figure 3-10. Sample comparisons of depth averaged along-channel velocity at three stations during three 1-month periods in 2012-2014. The averaged RMSE in 2012-2014 for all stations is 16 cm/s.
Figure 3-11: Vertical profiles of sub-tidal velocity at the Bay mouth (cb0102) and upper Bay (cb1101 and cb1201), with horizontal bars showing standard deviations.
3.4.3 Overall model skill for salinity and temperature

The performance of our model is similar to EPA’s regulatory model CH3D (Figure 3-7). The surface temperature is particularly well simulated, followed by the bottom temperature. The errors associated with the surface and bottom salinities appear to be smaller than other models. Not surprisingly, the two stratification indicators (the magnitude and the depth of the maximum vertical salinity gradient) have lower skill than those of the surface and bottom salinity. However, even with the lower skill associated with these variables, the model still performs better than the mean of the observations (represented by the unit circle). The RMSE’s for 3D salinity profiles are 1.8 PSU overall: 1.9 PSU for bottom salinity, and 1.5 PSU for surface salinity. The corresponding numbers for temperature are 1.4 °C, 1.6 °C, and 1.1 °C.

We also calculated the statistics for salinity and temperature in each year, and in the main channel and shallow shoals separately, which give similar skills as those in Figure 3-7. This suggests the model is capable of resolving temporal and spatial variabilities in these variables. Additionally, a transect along the main channel provides a more detailed view of the spatially variable, yearly averaged salinity structure (Figure 3-12; also refer to the station locations in Figure 3-1). The model generally captures the stratification structure and longitudinal salt transport well, with a small under-estimation at some lower Bay stations (e.g. CB7.4); an over-estimation of stratification in the mid-bay is also visible in 2012. In general, the model captures the spatial variability of stratification very well, including the local minimum near CB7.1S and CB5.5, and the largest stratification at CB3.3C. The maximum stratification at CB3.3C is due to its proximity to the freshwater zone and large depth (26 m) locally, and is generally modeled well.
Figure 3-12: Averaged salinity transect for 2011-2014 along the main stem stations. It overlays the observations (CBP casts) on top of the model results; complete ‘disappearance’ of the observation points indicates a perfect model.
3.4.4 Salinity

A complete assessment of the vertical structures using the 3D profiles is the most challenging for models. We present in Figure A1 (Appendix A) the model-data comparisons of CTD casts at eight representative stations in the main Bay. In these profiles, we used the best match within a 6-hour window (i.e. 3 hour before and after the actual time) to account for small phase errors in the model forcing; however, as in Ye et al. (2016), we found that the skill using the actual cast times are generally similar.

The comparisons at the five stations from lower Bay to upper Bay demonstrate that the model-data agreement is quite good (Fig. A1). Only marginal deterioration of skill is observed at the upper Bay stations like CB3.3C as compared to Ye et al. (2016). The strong stratification observed at CB3.3C and CB4.4 is generally well captured, but is under-estimated sometimes in summer low-flow seasons. The northern limit of the saltwater intrusion, as observed at CB3.1, is also accurately simulated by the model.

The profile comparisons at representative shallow shoal stations can be found in Figure A1. With adequate resolution used there, the model skill is similar to that in deep-channel stations. This is important, as increasing attention is being focused on these shallow productive areas.

3.4.5 Temperature

Modeled water temperature generally has a high skill (Figure 3-7 and A2), with an averaged RMSE of 1.4 °C and CC of 0.99. This suggests that the bulk aerodynamic module inside SCHISM (Zeng et al., 1998) works reasonably well. The seasonal variation is simulated well although the bottom temperature is sometimes over-estimated at some mid Bay stations (CB5.1), which seems consistent with the salinity error there and suggests the errors come from the same water mass. An important signal is observed in the lower Bay (e.g. CB7.4; Figure A2) due to coastal upwelling; the upwelled cold water resulting in drop in temperature at the surface.
and bottom is apparent at these stations during summer, under southeasterly (upwelling favorable) winds. The timing of these events seems to agree with satellite observations.

### 3.4.6 1996 survey

The dataset from this survey can be used to validate the model in the plume region under extreme forcings. The Chesapeake Bay plume is strongly influenced by the Bay outflow, bottom friction and wind, and the offshore extent of the plume is found between the scale predicted by geostrophic dynamics (internal Rossby radius) and the scale predicted by cyclostrophic dynamics (Valle-Levinson et al., 2007). Jiang and Xia (2016) discussed five types of plume structures as regulated by river outflow and wind.

The El Nino event in 1996 is one of the strongest in recent history, and was accompanied by large precipitation events in Feb, Sept, and Nov. 1996 (Figure 3-6b). The combination of the large outflow and upwelling favorable winds in Nov. 1996 pushes the freshwater plume ~90 km directly offshore (Figure 3-13a). The plume configuration roughly corresponds to Type II as described by Jiang and Xia (2016).

Note that the large offshore extent of the plume (Figure 3-13) is relatively rare for the Chesapeake Bay, as the plume seldom extends this far offshore due to the combined effects of Coriolis and the prevalent southward shelf current. The southward shelf current effectively arrests “upstream” intrusion of the plume, making it attached to the coast along the direction of Kelvin wave propagation (Fong and Geyer, 2002). This is very different from some other large river plumes that regularly spread far offshore (e.g. Columbia River).
Multiple transects near the Bay entrance were surveyed in September and November 1996 by Valle-Levinson et al. (1998, 2007) and the datasets serve as valuable information on the 3D structure of the Chesapeake freshwater plume. Here we present comparisons of velocity profiles along a few transects near the entrance collected during the surveys (the exact locations are shown in Figure 3-1). The profiles are temporally averaged over the 24-hour periods of each cruise (Valle-Levinson et al., 2007).

The model generally has a high skill in capturing the complex 3D flow in the plume region (Figure 3-14). The subtidal flow in Transects 2 and 3 revealed containment of the plume as
well as the outflow plume separating from Cape Henry resulting in a recirculation of bay plume there. These features are qualitatively captured by the model as well (Figure 3-14b).

Figure 3-14: Sub-tidal flows at each transect measured in September and November 1996. Looking upstream, shaded areas indicate up-estuary flow perpendicular to the transect; vectors indicate along transect (lateral) flow. The two panels are: (a) observation, redrawn from the data used in Valle-Levinson et al. (2007)’s Figure 6; (b) model results.
3.4.7 Model assessment on the shelf

Circulation patterns on the MAB continental shelf are driven by large-scale processes. The equatorward shelf current is the strongest signal on the inner shelf, while the poleward flowing Gulf Stream is dominant near the shelf break in the upper ~200 m. The Gulf Stream path veers towards the open ocean near Cape Hatteras where the current begins to transition from a topographically trapped western boundary current to a vigorously meandering free jet. Recent observations suggest that larger variability of this separation points may be a plausible cause for the warming of the MAB and local relative sea-level rise (Andres, 2016; Ezer, 2013). This baroclinic instability creates complex eddies and counter-currents between the Gulf Stream and the shelf currents (Chen et al., 2014a).

In the SCHISM model, we rely on HYCOM to provide the large-scale flows at the boundaries to bring in large-scale processes. Therefore, the model results near the ocean boundary are strongly influenced by HYCOM. We generally observed a smooth transition between the B.C. and the interior solution, suggesting that our B.C. and nudging approach works well. The monthly averaged surface currents from HF radar observations reveal large seasonal variability. The southward shelf current, the northward Gulf Stream and eddies in between are generally captured by the model (Figure A3). Superposed on these processes are the atmospheric forcing and freshwater outflow from the Bay that drive short-term variability. In general, the flow reversal on the inner shelf only occurs in the summer under southerly winds.

The averaged RMSE for the surface currents among all years is 18 cm/s. The higher resolution used in SCHISM nearshore allows us to better represent the details of flow structures particularly near the entrance to the Bay compared to the coarser resolution used in HYCOM, even though HYCOM uses data assimilation while our model does not (Figure A4). Away from the entrance the SCHISM results are strongly influenced by HYCOM, and thus sometimes inherit larger errors there (e.g. the Gulf Stream path as shown in Figure A4). This motivates us
to move the offshore boundary farther away from the Bay to reduce the influence from HYCOM; we will come back to this point in Chapter 4.

3.5 Discussion: importance of bathymetry

Numerous sensitivity tests conducted with SCHISM indicate that the high model skill is primarily attributed to (1) accurate representation of the bathymetry, particularly the channel profile, by the hybrid horizontal and vertical grids; (2) higher-order numerical methods developed in recent years (Zhang et al., 2016a; Ye et al., 2016). The importance of (1) will be further explained in this section.

A fundamental first-order forcing in shallow water regime is the underlying bathymetry. While the importance bathymetry in a numerical model is widely understood, the ideal is often compromised in practice. The reasons vary but here we distinguish two types of errors:

(a) Type I: representational errors due to bad values or the finite, discrete representation of the domain. Discretization will always result in errors in the representation of water depths and volume. There can be also be ambiguity over which quantities (point values or moments like face areas and volumes) are of higher priority and whether features like bed forms should be treated as sub-grid and modeled with closures or explicitly resolved.

(b) Type II: errors and adjustments harking back to artifacts of numerical models, including requirements for stability, accuracy or efficiency. These adjustments are often mandatory, in which case their deleterious effects may not be testable in a simple way.

Horizontal resolution is a remedy for many geometry-related issues, but any refinement below the scales of physical interest usually represents a computational expense that is hard to accept. Smoothing is also used in addressing bathymetry-related issues, although the role it
plays is different for the two types of errors enumerated above. An example involving representational difficulties (Type I error) would be the removal of small bathymetric features to avoid aliasing them on a coarser grid. The smoothing in this case may be coupled with a moment-preserving constraint such as volume preservation. Figure 3-15 shows an example taken from Liberty Island, an intertidal island in the Sacramento-San Joaquin Delta in California. The small-scale “moonscape” in this DEM arises mostly because of difficulties with bathymetry collection in a shallow, turbid and vegetated environment. The filtering algorithm used in (b) is due to Mallidi and Sethian (1996), based on an anisotropic curvature flow originally designed to de-noise features in medical images. This preprocessing step eliminates curvature below a specified length scale (in this case 20 m), but preserves steep slopes, peaks and valleys. Using a Nyquist analog as a rough guide, convergence in this case would be straightforward at scales from 40 m down to 10 m; any further refinement in the mesh would have to be reconciled with the choice of length scale of the smoother and the rough quality of the underlying data.

![Figure 3-15: An example of DEM smoothing: (a) original DEM in Liberty Island in Sacramento-San Joaquin Delta, showing small-scale “moonscapes” of a few meters; (b) smoothed DEM.](image)

More objectionable is the Type II case where bathymetry smoothing is required to make up for a shortcoming such as Pressure Gradient Errors (PGEs) in terrain-following coordinates,
first discussed by Haney (1991). In this case, a smoother is used to limit the coordinate slope, and in doing so it alters the bed geometry in systematic ways. The effects of Type II errors have not been carefully assessed so far because models based on terrain-following coordinates often become unstable without smoothing. Since SCHISM uses terrain-following like coordinate but is stable over non-smoothed bathymetry, we can systematically assess the error and false physics generated by the altered bathymetry.

We demonstrate with the current application case how bathymetry smoothing changes the character of the geometry in a way that leads to system-wide changes in response. In the sensitivity tests, the original bathymetry is smoothed inside different regions of the Bay-Shelf model using the Hannah-Wright smoother (Hannah and Wright 1995) with \( r = 0.1 \). Similar conclusion can be drawn for any smoother that fulfills a similar function, or with an \( r \) value as large as 0.8.

With the Hannah-Wright smoother, the depths at the vertices of each element are iteratively altered to satisfy the following criterion:

\[
\frac{h_{\text{max}} - h_{\text{min}}}{h_{\text{min}}} \leq r, \tag{3.1}
\]

or equivalently:

\[
h_{\text{max}} \leq (1 + r)h_{\text{min}}, \tag{3.2}
\]

where \( h_{\text{max}} \) and \( h_{\text{min}} \) are maximum and minimum depths in an element, and \( r \) is a user prescribed threshold related to the Haney criterion (usually on the order of 0.1). Eq. (3.2) could therefore be satisfied with a sufficiently fine resolution, at least in theory. If this criterion is violated in an element, the max/min depths are reduced/increased by an amount of \( 0.02*h_{\text{max}} \). The procedure conserves the original volume. The iteration continues until this criterion is satisfied by all elements, or the maximum depth change in two consecutive iterations is less than a prescribed threshold (e.g. 1 m).
In the rest of this section, we present two sensitivity tests in which the original bathymetry is smoothed in the mid-Bay and the whole domain respectively. We remark that (1) the baseline model is still subjected to Type I errors, but its bathymetry is much closer to the original DEM than the smoothed bathymetry used in the sensitivity test; (2) the sensitivity tests use the same parameters/forcing (except for the bathymetry) as the baseline model and are not recalibrated.

3.5.1 Local smoothing in a mid-Bay region

In the first sensitivity test, a region in the mid-Bay is smoothed (Figure 3-16a). As the volume is conserved by the smoother, the deeper channel becomes shallower, and the shallower shoals are deepened, with large bottom slopes removed (Figure 3-16: b versus c). These lead to changes in terms of mixing patterns, partition in volume flux, lateral flow, and the location of pycnocline. The sequence of this list of variables does not imply a cause-effect relationship, since they are interrelated components in a non-linear system and all governed by the underlying bathymetry. It should be noted the last variable is of particular interest in water quality and biological studies, since it is closely related to the hypoxic volume (Bever et al., 2013).

The most obvious change is seen in the mixing patterns (Figure 3-16bc). With the original bathymetry, large turbulence mixing is visible near the corners of the steep slope (Figure 3-16b); after smoothing, the mixing near the slope is reduced and the low mixing zone extends more into the shallows (the area highlighted by solid ellipses in Figure 3-16c). Note that the high-mixing zone near the corners is, in all likelihood, physical, and its absence in the smoothed bathymetry fortuitously masks numerical dissipation by lowering the amount of physical mixing. Even though the smoothing is only done in a small region in the mid-Bay, its effect is felt farther up-estuary. With smoothing, the salinity at CB3.3C increases by 1.6 PSU on average, because the total mixing (i.e., the sum of physical and numerical mixings) is kept low by under-
estimation of the physical mixing in the smoothed region. As a result, even low-order upwind scheme can apparently give ‘reasonable’ results for the averaged salinity, but not its 3D profile (because the original and altered depths do not even match). With the non-smoothed bathymetry used in our model, the higher-order schemes and the new LSC2 grid was previously shown to be essential for model accuracy (Ye et al., 2016).

The bathymetry smoothing also affects the partition of volume flux. Although the total volume flux across the entire transect (from bank to bank in Figure 3-16a) does not change (i.e. -1370 m³/s for both original and smoothed bathymetry, with negative values indicating seaward fluxes), the partitioning of fluxes between channel (the blue portion of the transect in Figure 3-16a) and shoal is altered as the channel volume is decreased and shoal volume is increased; the yearly averaged flux for the channel portion in 2012 is 74 m³/s (i.e. landward) for the original bathymetry and -197 m³/s (i.e. seaward) for the smoothed bathymetry, and the remaining fluxes for the shoal portion are -1444 m³/s and -1173 m³/s respectively. In other words, the channel-shoal contrast is reduced with the smoothed bathymetry. Under the original bathymetry, the intrusion occurs more along the channel and less along the shoal, resulting in more seaward outflow in shallow depths.

More importantly, the change in lateral salinity distribution results in a reduction in volume below pycnocline (defined as the location of the largest vertical salinity gradient; Figure 3-16d). After smoothing, the bottom high salinity intrudes more onto the shoal and the position of the pycnocline shifts. These lead to a 23.8% reduction in the area (along this transect) below pycnocline on average (up to a maximum of 49.6%). In other words, the hypoxic volume would be systematically underestimated with bathymetry smoothing. A more holistic view on the hypoxic volume in the Bay will be discussed in the next sensitivity test.

Lastly, several changes in the circulation patterns after smoothing are also noticeable (Figure 3-16e): (1) the lateral flow on the east side of the transect (20-40 km on the x-axis)
becomes more uniformly to the east; whereas more complex two-layer and even a three-layer exchange flows exist under the original bathymetry; (2) the lateral flow magnitude near the two land boundaries increases, which is likely due to the deepening of the shoal; (3) stronger exchanges occur near the channel slopes (near 14 km on the horizontal axis in Figure 3-16e) in the smoothed bathy; (4) longitudinal exchange flow is generally weakened (some surface flow near the two banks even changes the direction from seaward to landward ), with the core of the surface seaward flow moved on to the shoal. These suggest the cross-channel flow is highly regulated by the bathymetry; and bathymetry smoothing reduces channel-shoal contrast by artificially enhancing channel-shoal exchange.

Figure 3-16: Effects of bathymetry smoothing. (a): Smoothing region and the transect used in analysis; (b): time averaged (May-Dec, 2012) vertical diffusivity along the blue portion of the transect with the original bathymetry; (c): same as (b) but with the smoothed bathymetry. The dashed line in (b) shows the bottom profile from the original high-resolution DEM.
Figure 3-16 (continue): Effects of bathymetry smoothing in: (d) salinity distribution and pycnocline position; (e) flow patterns (arrows represent cross-channel flow and color represent along-channel velocity). All plots are time averaged from May to October in 2012.

3.5.2 Whole-domain smoothing

In the second sensitivity test, we apply the same bathymetry smoother on the entire model domain and focus on the overall system-wide changes. The most obvious change is that the Bay becomes saltier and more stratified after smoothing (with the same high-order transport solver) (Figure 3-17). This is due to a more ‘uniform’ intrusion pattern along the channel and the shoal (cf. insets of Figure 3-17). As a result, bathymetry smoothing often ‘helps’ models
with under-intrusion and under-stratification problems. However, since a first-order forcing (bathymetry) is altered to compensate errors in the simulated salinity etc., it is hard to reconcile it with other processes. For example, side channels are generally fresher and less stratified than the main channel. This is captured by the model with original bathymetry; an evidence is that the model skill on salinity is similar between the main channel stations and the side-channel stations (cf. Figure A1 for cast comparisons in the main stem and shallow regions), suggesting the shear dispersion is adequately captured. However, with the smoothed-bathymetry, although we could get a ‘similar’ intrusion in the main channel by using a lower-order transport scheme, the skill on side channel stations significantly deteriorates. This is because the channel-shoal difference in salinity is reduced and the model is no longer able to capture the spatial heterogeneity in the lateral salinity distribution. In the rest of this sub-section, we first examine the change in intrusion pattern by a salt budget analysis, followed by a discussion on its implications on other key variables.

Figure 3-17: Simulated stratification (bottom salinity minus surface salinity, time-averaged in 2012): (left) original bathymetry; (right) smoothed bathymetry (with the same transport solver). Note that the zoomed-in views use a range of 0-1 PSU to mark the intrusion limit.
Salt budget

Salt budget is analyzed on several cross-channel transects from the Bay mouth to the upper Bay (Figure 3-18). Following Lerczak et al. (2006)’s procedure, the total flux is defined as:

$$F_s = \langle \int u s \, dA \rangle,$$  \hspace{1cm} (3.3)

where \(u\) is the velocity component perpendicular to the transect; \(s\) is salinity; \(A\) is cross-sectional area. We first decompose a generic variable \(\phi\) into sub-tidal and tidal components:

$$\phi_0 = \frac{1}{A_0} \langle \int \phi \, dA \rangle,$$

$$\phi_E = \langle \frac{h + \eta}{h} \phi \rangle - \phi_0,$$  \hspace{1cm} (3.4)

$$\phi_T = \phi - \phi_0 - \phi_E,$$

where \(A_0\) is sub-tidal cross-sectional area; \(h\) is bathymetry depth; \(\eta\) is the tidally fluctuating surface elevation. \(F_s\) is then approximately decomposed into:

$$F_s = \langle \int (u_0 + u_E + u_T)(s_0 + s_E + s_T) \, dA \rangle$$

$$\approx \langle \int (u_0 s_0 + u_E s_E + u_T s_T) \, dA \rangle \equiv Q_f s_0 + F_E + F_T,$$  \hspace{1cm} (3.5)

where \(F_s\) is the total salt flux; \(Q_f s_0\) includes the salt flux from both river discharge and Stokes transport; \(F_E\) is the salt flux from subtidal shear dispersion; and \(F_T\) is the tidal oscillatory salt flux. As shown in Figure 3-18, the difference in total salt flux \((F_s)\) between the two bathymetries grows rapidly from the mouth to the upper Bay, with a sign reverse at both the mid-Bay transect and the upper Bay transect after smoothing. The flux decomposition shows that the estuarine circulation flux \((F_E)\) is the major contributor to this discrepancy, whereas the salt flux from river discharge and Stokes transport \((Q_f s_0)\) and the tidal oscillatory flux \((F_T)\) play minor roles.
In particular, $F_E$ is mostly larger inside the Bay after smoothing, and the change in $F_T$ becomes larger in the upper Bay.

![Salt flux decomposition](image)

Figure 3-18: Salt flux decomposition ($F_s \approx Q_s s_0 + F_E + F_T$) at three cross-channel transects passing through CB7.4C (mouth), CB4.4 (mid-bay), and CB3.3C (upper bay) respectively (see exact locations in Figure 3-2), with comparisons between original and smoothed bathymetry. The time period is Oct-Dec, 2012.

**Hypoxic volume**

The averaged below-pycnocline volume in 2012 is reduced by 33.7% with the smoothed bathymetry, which is consistent with the results in Section 3.5.1. In addition, the distribution of this volume between channel and shoal is very different (cf. Figure 3-16d). This has significant implication for the estimate of summer hypoxia.

**Bottom stress**

The simulated bottom stress under the original and smoothed bathymetry is shown in Figure 3-19. With the original bathymetry, the bottom stress shows a channelized pattern. In many locations, the main channel is recognizable through a lateral contrast of bottom stress. This pattern is greatly smeared out in the smoothed bathymetry, and the bottom stress shows more of a longitudinal contrast rather than a lateral contrast, with little channel-shoal difference. Overall, the bottom stress patterns have more features under the original bathymetry that can
be related to the bathymetry. Obviously, these changes will lead to large differences in the simulated sediment dynamics.

![Image](image_url)

Figure 3-19: Simulated bottom shear stress on: (left) original bathymetry, and (right) smoothed bathymetry.

**Plume extent**

We define the plume volume as the water volume outside the Bay mouth enclosed by the 30-PSU iso-surface. Large differences (up to 52%; Figure 3-20a) are found in plume volumes between the two sets of bathymetries. However, the monthly trend shows a more complex picture (Figure 3-20a). During the spring freshet, the plume is much larger on the smoothed bathymetry, whereas it is slightly smaller during the low-flow season (Figure 3-20a). In other words, the ‘original’ plume shows less variability. Not surprisingly, the largest difference
corresponds to the largest plume extent during freshet (Figure 3-20ab). From the mass conservation point of view, a stronger salt intrusion (especially during freshets) under the smoothed bathymetry is generally compensated by a larger coastal plume, with a fresher bulge located farther offshore (Figure 3-20a).

![Figure 3-20: Difference in the simulated plume between the original bathymetry and the smoothed bathymetry: (a) time series of plume volume and percentage change after smoothing; (b & c) plume thickness in two representative months for (b) spring freshet and (c) low flow conditions in 2012. Note that the horizontal extents are different in (b) and (c). The plume areal extent is delineated by the 0 contour line.](image)

**Influence of horizontal resolution**

Based on the two sensitivity tests above, we believe bathymetry smoothing (and in general Type II errors) should be avoided as much as possible, especially in estuarine/nearshore applications. As the Haney criterion is a function of the horizontal grid size, the question might be asked whether it is possible to avoid bathymetry smoothing without violating the Haney criterion by refining the horizontal grid. We’ll use the high-resolution DEM for the Bay to estimate the horizontal resolution required to satisfy Eq. (3.2). The results indicate that: along the channel edges (at ~20 m depth), 90% of the bottom slopes are steeper than 0.5, 30% steeper...
than 1, with an average slope of 0.9 and the maximum slope of 8.9. These numbers are typical in many estuaries, partially due to maintenance dredging. Therefore, assuming a Hannah-Wright ratio of $r=0.1$, we can demonstrate that the horizontal grid resolution needs to be finer than ~6.5 m at a slope of 0.3, ~2.1 m at a slope of 0.9, and ~0.23 m at the maximum slope of 8.9. Even with an optimistic value of $r=0.8$ (estimated with ROMS), the resolution is still too fine. Obviously, this kind of resolution is very difficult to implement even with the help from high performance computers; in addition, it also puts a very stringent time step limit if the model is explicit. Resolving the channel-shoal contrast in realistic applications is therefore beyond the capability of most existing models.

Of course, many of our comments assume the availability of an elevation map of sufficient quality and resolution, usually much finer than the numerical grid. A coarser DEM causes feature loss analogous to that of isotropic smoothing. Fine-scale bathymetry, on the other hand, reveals steep bottom slopes as the grid is refined, exposing flow processes that may be of physical interest but also making it more difficult to satisfy the Haney criterion. We regard modeling these features as a positive thing, but there is one caveat that the continuous revelation of finer scales may at some point interfere with convergence, unless a length scale limitation is applied when extracting fine-scale features from the DEM.

3.6 Ocean B.C.

Previous studies did not give a clear answer to the influence of the ocean B.C. on the Bay processes. Here we examine the influence using two types of B.C.’s: HYCOM and monthly climatology.

It’s obvious that using the monthly climatology of temperature as B.C. would not resolve the inter-annual variability which is important for this variable, while the inter-annual variability in the ocean salinity is much smaller. We therefore used HYCOM temperature and
salinity climatology as our B.C. and nudging target near the ocean boundary. Sensitivity tests using HYCOM salinity as the B.C. revealed that the salinity in the Bay is mostly close to that from the climatology, but sometimes with 1-2 PSU over-estimation at the entrance (Figure 3-21). As CB7.4 effectively acts as a ‘B.C.’ to the rest of the Bay, similar errors are propagated into upstream stations. It seems that HYCOM occasionally over-estimates the ocean salinity but there is no clear seasonal trend for this bias. Scarcity of observation in the ocean makes it hard to systematically assess HYCOM skill there.

Note that inter-annual variation in the ocean salinity may not be negligible especially under future climate change. This motivates us to further enlarge our domain in order to mitigate the effects of B.C. Even though the model does not use data assimilation (as in HYCOM), the hope is that the model bias would be easier to interpret and one could potentially obtain a better estimate of the ‘B.C.’ at the Bay entrance.

An alternative approach used by other models (e.g., the EPA operational model based on CH3D) is to place the open boundary near the entrance. This, however, may cause issues in capturing the complex flows near the boundary (cf. Section 3.4.6). In addition, the temporal resolution of the observed T/S time series at CB7.4 is not high enough to resolve the tidal signal.

Besides B.C., we have also conducted extensive sensitivity tests with respect to other forcing and model parameters. We found that using the river flow from the measured daily discharge values at the 7 major tributaries instead of the watershed model generally yields similar results but with a slightly lower overall skill. Consistent with the findings in Ye et al. (2016), the use of TVD$^2$ and the hybrid NARR wind appreciably improves the model skill.
Figure 3.21: comparison of bottom salinity at (a) CB7.4 and (b) CB3.2 calculated from using climatology and HYCOM as B.C. The shaded regions correspond to the ranges of the bottom observation depths, which vary through time.

3.7 Conclusions

We have successfully applied a 3D baroclinic unstructured-grid model to Chesapeake Bay and the adjacent continental shelf. Recently developed new methods (TVD^2, LSC^2 and hybrid triangular-quadrangular grid) are used in this cross-scale application. We showed that the model is both accurate and efficient for this system. The sea-surface elevation is particularly well simulated. The velocity, salinity and temperature and their vertical structures are also well captured by the model. The new model is very flexible in its horizontal and vertical grids, and thus can be easily extended into tributaries and sub-tributaries.

We demonstrated the fundamental importance of bathymetry representation in the estuarine and nearshore models. Bathymetry smoothing commonly used in terrain-following coordinate models was shown to not only lead to consistency issues, but also fundamentally alter the system in terms of volumetric and tracer fluxes and channel-shoal contrast.

The proper representation of the physical processes is a pre-requisite for water quality and biological studies in the Chesapeake Bay and elsewhere. Therefore, the model presented
in this chapter represents a powerful tool that can be used to advance our understanding of the impact of both local and remote forcings on estuarine systems, which can ultimately lead to a holistic management strategy.
4 Large domain: Third-order transport schemes for unstructured-grid model in the eddying regime

Abstract

Despite the recent success achieved by our unstructured-grid (UG) model in multi-resolution coastal studies, its skill in the adjacent eddying ocean still needs improvement before its cross-scale potential can be fully realized. One of the reasons that UG coastal models often lack skills in the eddying regime is that the transport schemes developed for estuarine settings are too dissipative in the eddying regime. To fill this gap, this chapter presents a 3rd-order transport scheme based on Weighted Essentially Non-Oscillatory (WENO) formulation, aimed at better resolving meso-scale features in the eddying regime. In particular, we choose a design that maintains accuracy for coastal ocean applications, while optimizing monotonicity, efficiency, and robustness in the eddying regime. We demonstrate with several numerical benchmarks that the new scheme reduces numerical diffusion and better captures eddies and filaments associated with baroclinic instability. A preliminary application to the Gulf Stream shows that the new scheme better resolves the meso-scale eddies and meanderings than a 2nd-order scheme that is considered sufficient in an estuarine setting. These results confirm the necessity of high-order transport schemes for the eddying regime, and represent a key step in our ultimate goal of developing a bona fide cross-scale UG model for the Chesapeake Bay.

4.1 Introduction

Unstructured-grid (UG) models have seen increased applications over the past two decades, mainly due to its flexibility in (1) resolving bathymetric and geometric features, and (2) local refinement/de-refinement for the area or process of interest/disinterest. A key challenge for UG model development is to fully realize its potentials in cross-scale problems. A review by
Danilov (2013) indicates that until recently large-scale ocean applications are still lacking in the UG model community. In fact, the baroclinic applications of UG models are mostly confined to coastal regions (Chen et al., 2003, Fringer et al., 2006, Zhang and Baptista 2008). Recently, much progress has been made by a triad of global UG models (FESOM (Wang et al., 2014), MPAS (Ringler et al., 2013) and ICON (Korn, 2017)) in simulating global-scale processes with eddying permitting and resolving capability. Different from the coastal models, the designs of these UG models are aimed at simulating the global ocean circulation, thus leaving gaps between their finest resolvable (capped by computational cost) ocean dynamics and the even finer scale coastal processes. One example of such design is the Spherical Centroidal Voronoi Tessellations used in MPAS-Ocean, which handle multi-resolutions well for the more regularly shaped deep ocean, but are still not cost-effective in resolving highly irregular geometries in estuaries and coastal regions. In fact, we are engaged in an ongoing project funded by the Department of Energy (DOE) to couple an UG coastal model to the global MPAS-Ocean model.

This motivates us to extend our coastal model domain further into the deep ocean. There are two benefits from this endeavor as far as model coupling is concerned: (1) for the global ocean model, its scale contrast can be reduced, which not only reduced the size of the computational grid, but more importantly increases the maximum allowable time-step because the most stringent CFL condition is generally associated with the finest grid resolution; (2) for the coastal model, the uncertainties from the ocean boundary conditions (B.C.) can also be reduced. For example, in our recent study on the Chesapeake Bay we observed errors that most likely came from the ocean boundary conditions derived from the global HYCOM (Figure 4-1a). Even though the model boundary was set 100 km beyond the shelf break and 200 km from the Chesapeake Bay mouth, the effect from the ocean B.C. can still be seen at the mouth
The presence of the meandering the Gulf Stream core in this region further complicates the treatment of B.C. (Fig. 4-1a-c).

Our goal in this chapter is to enhance our UG model’s capability in the eddying regimes. Previously, higher-order momentum advection schemes with stabilization schemes using viscosity/filters have been developed in Zhang et al. (2016a) to address the issue of spurious mode. However, we find that meso-scale eddies and meanders tend to be under-resolved using the 2nd-order transport schemes that are considered sufficient for estuarine applications. This is

Figure 4-1: Model error in SST possibly inherited from the ocean boundary conditions: (a) observation; (b) SCHISM model results; (c) HYCOM product used to force the ocean boundary condition in SCHISM; (d) the effect of the ocean boundary conditions on the simulated salinity at the Chesapeake Bay mouth (station CB7.4 in (a)).
likely because the intrinsic physical dissipation is large in estuaries due to bottom friction and strong mixing, which may effectively mask numerical dissipations (we have discussed in Chapter 3 that bathymetry smoothing further lowers the simulated ‘physical’ dissipation, thus allowing even higher inherent numerical dissipation). In an eddying ocean, however, the forces are largely balanced (Ringler et al., 2013) and physical dissipation is at a much lower level, and therefore the numerical dissipation needs to be carefully controlled. Higher-order transport schemes are generally thought to be necessary in the eddying regime.

For our purpose, we seek a transport scheme that is (1) easily extendable to 3rd or higher order accuracy; (2) monotonic or nearly so; (3) robust on generic unstructured grid (without geometric constraints, such as orthogonality or mesh quality). Third-order schemes are generally considered optimal because the leading order truncation errors are in the form of diffusion instead of dispersion, thus greatly reducing the need for the use of additional explicit diffusion to avoid unphysical oscillation. The second requirement on monotonicity is also important. For example, the distribution of dissolved substances may have large gradients in nearshore or deep ocean, which may trigger unwanted numerical oscillations. Although various filtering techniques have been proposed before (Shchepetkin and McWilliams, 2005), they are not ideal since they reduce effective order of convergence. The third requirement on robustness is intended for easy transitioning between more uniform grid in the ocean and more irregular grid as common in the coastal region. We found the weighted essentially non-oscillatory (WENO) scheme satisfies these requirements well.

Introduced by Liu et al. (1994), the WENO scheme has been applied in various fields including computational fluid dynamics, astrophysics, biology, etc.; the review by Shu (2009) provides a comprehensive list of related applications. In the field of ocean modeling, it has been adopted by the SG model ROMS for the sediment transport in the vertical dimension (Warner et al., 2008). After its extension to UGs (Friedrich, 1998; Hu and Shu, 1999), WENO
has also attracted attentions from the UG practitioners especially in the field of morphodynamics (Canestrelli et al., 2010; Guerin, Bertin and Dodet, 2016). To our knowledge, WENO has not been applied to the horizontal tracer transport for UG modeling in the eddying regime.

In this chapter, we present a numerical method based on WENO formulation for the horizontal transport in our UG model, with an aim to better resolving meso-scale eddies and meanders in the eddying regime. The following text is structured as follows: in Section 4.2, we first briefly summarize the discretization of transport equation in SCHISM, then explain the challenges when adapting WENO to our model and how we design the FV solver accordingly. Section 4.3 presents the results from a few benchmarks including a rotating Gauss Hill test and a reentrant channel test. Then in Section 4.4, we present a preliminary application to the Gulf Stream, and compare the performance between the new scheme and a TVD scheme. With these tests and applications, we also discuss the limitations of the new scheme and potential improvements in the conclusions (Section 4.5).

4.2 Methods

4.2.1 Operator splitting

The operator splitting procedure was previously discussed in Section 2.2.1, so the details will not be repeated here except for some key steps. Starting from the transport equation (Eq. (2.1)):

\[
\frac{\partial T}{\partial t} = -\nabla \cdot (uT) + \frac{\partial}{\partial z} \left( \kappa \frac{\partial T}{\partial z} \right) + q,
\]

we utilize a finite volume framework (Figure 4-2) and obtain its discretized form (Eq. (2.7)):

\[
T_{i}^{n+1} - T_{i}^{n} = -\frac{\Delta t}{V_i} \left\{ \sum_{j \in S^-} \left[ |Q_j| (T_j - T_i) \right] + \sum_{j \in S^+} \left[ |Q_j| \Phi_j \right] - \sum_{j \in S^-} \left[ |Q_j| \Phi_j \right] \right\}
\]
\[ + \frac{\Delta t}{V_i} \left[ \left( \kappa'_j \frac{\partial T_j}{\partial z} \right)_{j=i+1} - \left( \kappa'_j \frac{\partial T_j}{\partial z} \right)_{j=i-1} \right] + \frac{\Delta t}{V_i} \int q, \]

where \( T \) represents the concentration of a generic tracer defined at prism centers (or more precisely, average concentration in a prism); \( q \) includes all source and sink terms; \( \mathbf{u} \) is the three-dimensional velocity vector \((u, v, w)\) (m s\(^{-1}\)); \( T' \) is concentration at a face of the prism, which will be reconstructed from prismatic concentration \( T \) in subsequent steps; \( i \) is a prism index; \( j \) is a face index; \( n \) is time level; \( V_i \) is the volume of Prism \( i \); \( Q \) (positive leaving Prism \( i \)) is the volumetric flux through each face, which has already been solved by the momentum equation at the current step; \( \kappa' \) is vertical diffusivity defined at top or bottom faces of the prism.

We use \( S \) to denote all prism faces including inflow faces \( S^- \) and outflow faces \( S^+ \). Additional symbols of vertical levels are introduced for convenience: \( i^+ \) is the prism on top of prism \( i \); \( i^- \) is the prism below prism \( i \); \( i \cap i^+ \) is the top face of prism \( i \); \( i \cap i^- \) is the bottom face of prism \( i \); \( \Phi \) is a generic correction term to achieve higher order. The time levels of \( T \) on the right-hand side (RHS) will be specified next.

Vertical levels

\[ \bullet i + 1 \]

\[ \bullet i \]

\[ \bullet i - 1 \]

\[ \text{Figure 4-2: Two types of prisms as the control volumes in SCHSIM transport. Tracer concentrations are defined at prism centers. Face concentrations will be reconstructed from prism center concentrations.} \]

Previously, the transport equation (2.2) was split into 3 steps: horizontal advection (Eq. (2.8)); vertical advection (Eq. (2.9)); and other terms (Eq. (2.10)). Here, we revisit Eq. (2.8)
and substitute the previously implemented 2\textsuperscript{nd}-order TVD scheme with a 3\textsuperscript{rd}-order WENO scheme. To conform to the generic form of Eq. (2.4), where a higher-order approximation is achieved by adding a correction term \( \Phi \) to the upwind approximation, we trivially set:

\[
\begin{align*}
\Phi_j &= T'_j - T_j, \quad j \in S^- \\
\Phi_j &= T'_j - T_j, \quad j \in S^+
\end{align*}
\]

and obtain the WENO-based horizontal advection scheme:

\[
T_i^{(1)} - T_i^n = -\frac{\Delta t}{V_i} \left\{ \sum_{j \in S^-} [Q_j(T_i - T_j)] + \sum_{j \in S^+} [Q_j(T'_j - T_i)] - \sum_{j \in S_H} [Q_j(T'_j - T_j)] \right\},
\]

which is equivalent to

\[
T_i^{(1)} - T_i^n = -\frac{\Delta t}{V_i} \left\{ \sum_{j \in S_H} [Q_j(T'_j - T_i)] \right\},
\]

since we have defined \( Q_{j \in S^-} < 0 \) and \( Q_{j \in S^+} \geq 0 \). Because Eq. (4.3) is an explicit scheme, the time step is limited by:

\[
\Delta t \leq \frac{V_i}{\left| \sum_{j \in S_H} Q_j \right|} \mathcal{C},
\]

where \( \mathcal{C} < 0.5 \) is the CFL number for finite-volume schemes on 2D (Toro, 2013).

4.2.2 WENO design

The transport solver designed here caters to cross-scale estuarine/ocean baroclinic applications on generic unstructured grids, and is suitable on parallel machines. For this purpose, we consider the following specific needs: (1) third-order accuracy is necessary and potential extension to fourth-order is possible; (2) violations in monotonicity should be kept minimal, preferably without adding artificial diffusion; (3) simple stencils are preferred to maintain the
parallel efficiency; (4) the algorithm should be robust for all grid configurations as found in oceans and estuaries. These considerations are reflected in the procedure described below.

**Numerical flux and stencils**

A key step in WENO procedure is to reconstruct the interfacial mass flux (the term between brackets in Eq. (4.3)). Following Hu and Shu (1999), the mass flux $Q_j T'_j$ can be approximated by a $q$-point Gaussian integration formula:

$$Q_j T'_j = Q_j \sum_{k=1}^{q} T(x^{G_k}, y^{G_k}), \quad (4.5)$$

where $q = 1$ is chosen (i.e., a single point at the side center; subscript $k$ is dropped in the subsequent text), since we only need 3rd-order accuracy in the final scheme. Should there be a need to go to 4th-order, two quadrature points per side would be needed. Note that the interfacial volume flux $Q_j$ is taken out of the summation on the R.H.S. of Eq. (4.5), because it is independent of tracer concentration and treated as constant on face $j$. For simplicity and efficiency, the upwind flux is used for $Q_j T'_j$, which seems sufficient for our purpose; in the future, we will examine the cost-effectiveness of other fluxes, such as Lax-Friedrichs, Rusanov, Roe, etc. (Toro, 2013).

For each quadrature point $(x^G, y^G)$, a set of stencils are needed to build polynomials, which relate prismatic values to the quadrature point. Since we are using the upwind flux, these stencils are centered on the upwind prism of $(x^G, y^G)$. We choose the “Tier-1” neighborhood as defined by the elements that share 1 or 2 nodes with the center element (Figure 4-3). The stencil candidates are constructed by sequentially listing the elements in this neighborhood in the counter-clockwise fashion, starting from the centering element. For a linear polynomial reconstruction, known values from 3 elements are required to determine its coefficients, and potential choices are 0-1-2, 0-2-3, ..., etc.; for a quadratic polynomial, at least 6 elements are
required, and potential choices are: 0-1-2-3-4-5, 0-2-3-4-5-6, …, etc. This neighborhood is
generally sufficient for constructing quadratic polynomials that lead to 3\textsuperscript{rd}-order accuracy; it
also simplifies the MPI communication. Our experience suggests that Tier-1 stencils are
generally less prone to oscillations than Tier-2 stencils (i.e. Tier-1 elements plus their Tier-1
neighbors).

To reduce truncation error, normalized local coordinates are used on each stencil, such that
(1) the coordinate origin coincides with the centroid of the centering element; (2) the $x$ and $y$
axes are scaled (without rotation) by a same factor, i.e. the largest distance between the origin
and the centroid of any neighboring elements in the current neighborhood. Then, the value at
the quadrature point is reconstructed by a linear combination of the approximated values from
each polynomial/stencil:

$$T(x^G, y^G) = \sum_{s=1}^{N_s} w_s p^n_s (x^G, y^G),$$

(4.6)

where $s$ is the index of all stencils centered on the upwind element of the current side; $N_s$ is the
number of stencils; $w_s$ is the weight; $p^n_s$ is an $n$-th order polynomial based on the $s$-th stencil.
The polynomials in Eq. (4.6) are exact at element centers and $(n + 1)$-th order accurate
elsewhere; moreover, it is possible to achieve $(n + 2)$-th order through an optimal choice of
the weighting $w_s$ (Hu and Shu, 1999).
Weights

We decide to not apply the weight optimization procedure as described in (Hu and Shu, 1999). The rationale is that 3rd order accuracy is sufficient for our applications; more importantly, optimal weighting is not always guaranteed in a generic UG. Liu and Zhang (2013) proposed a reconstruction that uses optimal weights in normal cases and reduces to lower-order in abnormal cases. We might adopt their method should there be a need to go to 4th order in the future. Since we are currently not applying optimal weighting, the weights $w_s$ are solely determined by the gradient of the concentration field within the current stencil:

$$w_s = \frac{\tilde{w}_s}{\sum_{s=1}^{N_s} \tilde{w}_s}, \text{with } \tilde{w}_s = \frac{1}{(\varepsilon + IS)}.$$  (4.7)
where $\epsilon$ is a small number to prevent division by zero. We find $\epsilon = 10^{-5} - 10^{-7}$ generally works well for the 3rd-order scheme, with only minor oscillations that can be safely ignored, whereas an $\epsilon$ larger than $10^{-4}$ tends to generate larger oscillations near tracer gradients. The choice of the smoothness indicator ($IS$) follows Hu and Shu (1999)'s formulation. For linear stencils used in 2nd-order schemes, the smoothness indicator is:

$$IS = \frac{1}{A} \int \left[ \left( \frac{\partial p}{\partial x} \right)^2 + \left( \frac{\partial p}{\partial y} \right)^2 \right] dS,$$

(4.8)

where $A$ is the area of the centering element, $\int dS$ is an integration over the area of the centering element. For a quadratic stencil leading to a 3rd-order reconstruction, the smoothness indicator is:

$$IS = \frac{1}{A} \int \left[ \left( \frac{\partial p}{\partial x} \right)^2 + \left( \frac{\partial p}{\partial y} \right)^2 \right] dS + \int \left[ \left( \frac{\partial^2 p}{\partial x^2} \right)^2 + \left( \frac{\partial^2 p}{\partial x \partial y} \right)^2 + \left( \frac{\partial^2 p}{\partial y^2} \right)^2 \right] dS.$$

(4.9)

We use the 3rd-order reconstruction based on quadratic polynomials by default, but revert to 2nd-order reconstruction in abnormal cases.

**Abnormal cases**

The use of generic unstructured grid can lead to abnormal cases, which have to be handled to ensure robustness. One of them is related to the availability of linear/quadratic polynomials. Figure 4-4 illustrates an invalid stencil for constructing a linear polynomial (2nd-order reconstruction), where the three element centroids are co-linear, which causes singularity in the matrix inversion associated with the linear reconstruction. A similar invalid case for the 3rd-order reconstruction is shown in Figure 4-6b. To identify near-singular stencils, we compute the determinant of the matrix in the normalized coordinates mentioned earlier, and remove stencils with a normalized determinant smaller than a prescribed threshold (e.g. $10^{-3}$).
Another abnormal case is related to the so-called “straddling stencils” being the only choices in the reconstruction procedure. Figure 4-5 shows straddling stencils vs. non-straddling stencils with respect to a particular face where the quadrature point is located. Suppose Element 2 is downwind of Element 0, and we want to reconstruct the value at Face 0-2 (interface between Element 0 and Element 2). Some stencil candidates may have elements lying on both sides of that face (e.g., Stencil 0-2-3 in Figure 4-5a), and may induce oscillations if there is a shock across Face 0-2, and in this case the WENO procedure would assign a small weight to this stencil according to Eq. (4.7). On the other hand, other non-straddling stencils (e.g., Stencil 0-9-10 in Figure 4-5b) would be given larger weights under such a case. Having stencils that cover all directions from the centering element is therefore ideal to prevent oscillations (Hu and Shu, 1999). However, this may not always be possible for generic UGs. For example, the number of available choices for 3rd-order stencils is limited on a uniform quadrangle mesh (Figure 4-6). In this case, for any given side of the centering element, the candidate stencils are either straddling it (Figure 4-6a shows two such cases) or singular (Figure 4-6b). As a result, all non-singular stencils will be given a similar weight by Eq. (4.7) even if their IS’s are large, which leads to excessive numerical dispersions. A straightforward remedy for such a situation is to downgrade to 2nd-order stencils, which only require 3 elements and so more choices are available. This is not against our objective in improving model skill in the eddying regime, since triangles are typically used in the regular-shaped open ocean, whereas quadrangles are mostly used to resolve channels inside estuaries, for which 2nd-order accuracy is sufficient.
Alternatively, we can use Tier-2 neighborhood for quadrangular elements to obtain 3\textsuperscript{rd}-order accuracy; this is not done at the moment.

![Linear stencils](image)

**Figure 4-5:** Linear stencils (blue and red elements) centered on Element 0: (a) a stencil with elements on both sides of Face 0-2 (dashed yellow line), i.e., a straddling stencil for Face 0-2; (b) a stencil with all its elements on one side of Face 0-2 (dashed yellow line).

![Exceptional case](image)

**Figure 4-6:** An exceptional case with a uniform rectangular mesh, where reconstruction based on quadratic polynomials is impossible because all candidate stencils are either (a) straddling a same side or (b) singular.

**Boundary conditions**

As illustrated in Figure 4-7, special treatments are applied at both the boundary sides (with two nodes on the boundary) and the near-boundary sides (with only one node on the boundary). The treatment of land boundary sides is straightforward, as no-flux condition is imposed and thus no reconstruction is required there. For open boundary sides, the inflow case and outflow case are treated separately. The inflow side values are relaxed to observation or other large-
domain model results, whereas the outflow sides take the values of the upwind prisms. For near-boundary sides, at most 2\textsuperscript{nd}-order accuracy is applied since a higher-order accuracy stencil is generally not available due to geometric constraints near the boundary.

![Diagram of boundary treatment for the WENO-based transport in SCHISM.]

Figure 4-7: Boundary treatment for the WENO-based transport in SCHISM.

### 4.3 Numerical Experiments

#### 4.3.1 Rotating Gauss hill

We conduct a rotating Gauss hill test to compare the new scheme based on 3\textsuperscript{rd}-order WENO with other lower order schemes. The test uses a solid body rotation as flow field with passive tracers in the form of a Gauss hill, so that the transport solver can be tested in isolation from the momentum and continuity equations. The test domain is a circular 2-D disk with a radius of 3600 m. The rotating flow field is defined as

\[
\begin{align*}
u &= -\omega y; \\
v &= \omega x,
\end{align*}
\]

with the angular velocity \( \omega = 2\pi/3000 \) (rad s\(^{-1}\)), i.e., one rotation per 3000 seconds. The initial concentration (Figure 4-8a) is in the form of a radially symmetric Gauss hill with the maximum concentration at the center \((x_0, y_0)\):
where $x_0=0$ m, $y_0=1800$ m, and $\sigma=850$ m. The domain is discretized by essentially uniform triangles using DistMesh (Persson and Strang, 2004). The 3rd-order WENO scheme is compared to the 1st-order upwind scheme and the 2nd-order TVD scheme. The maximum Courant number is chosen as 0.05 for all schemes. It is seen that the shape of the Gauss hill is nicely preserved by the 3rd-order WENO scheme (Figure 4-8e,f); even with a low resolution of 400 m (Figure 4-8d), it is comparable to upwind results with a much higher resolution of 100 m (Figure 4-8b). The higher accuracy of WENO is achieved at the cost of a 30% increase in computational cost compared to the TVD scheme (Table 4-1). Both upwind and TVD schemes, which are based on quasi 1D reconstruction (i.e. neglecting the cross-wind direction), are susceptible to grid orientation; whereas the WENO scheme, which uses a truly multi-dimensional reconstruction, is not (Figure 4-8).

Table 4-1: Comparison of different schemes in the Gauss hill test with $\Delta x=100$m.

<table>
<thead>
<tr>
<th></th>
<th>Upwind</th>
<th>TVD</th>
<th>WENO</th>
</tr>
</thead>
<tbody>
<tr>
<td>RMSE</td>
<td>0.035</td>
<td>0.017</td>
<td>0.002</td>
</tr>
<tr>
<td>Over/under-shoots</td>
<td>0/0</td>
<td>0/0</td>
<td>0/-2×10^{-5}</td>
</tr>
<tr>
<td>CPU time relative to TVD</td>
<td>0.8</td>
<td>1</td>
<td>1.3</td>
</tr>
</tbody>
</table>
Figure 4-8: Gauss Hill test: (a) initial concentration; (b) Upwind scheme on a fine mesh; (c) TVD scheme on a fine mesh; (d)-(f): the 3rd-order WENO scheme results after one rotation on progressively finer meshes.
4.3.2 Reentrant channel

The reentrant channel test case is a simple benchmark test for assessing model performance on baroclinic instability (Danilov 2012; Zhang et al., 2016a). The domain is a rectangular zonal band from 180ºW to 180ºE and between 30ºN and 45ºN, with a depth of 1600 m. The salinity is kept at 35 PSU throughout the simulation. The initial temperature is linearly varying along the vertical and meridional directions, with a small amount of ‘noise’ along the zonal direction in order to speed up the development of baroclinic instability (Danilov 2012):

\[ T_0(\lambda, \phi, z) = 25 + \alpha_1 z + \alpha_2 (\phi - \phi_0) + \alpha_3 (2\pi \lambda / L_0), \]  

(4.12)

where \( \alpha_1 = 8.2 \times 10^{-3} \text{C/m} \), \( \alpha_2 = -0.5566 \text{C/(degree latitude)} \), \( \alpha_3 = 0.01 \text{C} \), \( \phi \) is the latitude, \( \phi_0 = 30^\circ \text{N} \), and \( \lambda \) is the longitude, and \( L_0 = 20^\circ \). The flow is forced by relaxing temperature to its initial distributions within two 1.5º-wide southern (lower) and northern (upper) relaxation zones near the solid boundaries there.

This test was previously conducted in the SCHISM paper (Zhang et al., 2016a), where we made the comment that the filaments resolved by SCHISM were slightly shorter than the best results achieved in the original test by Danilov (2012), suggesting slightly larger numerical dissipation. From the comparison of temperature between the old and new schemes in Figure 4-9, we can see a large part of the numerical dissipation is indeed related to the TVD tracer transport scheme. With the new WENO scheme, longer filaments (Figure 4-9ab) and stronger vorticities (Figure 4-9cd) are generated. Consistent with the temperature pattern, the 3rd-order WENO scheme also leads to an increase of 10.1% in the simulated mean kinetic energy.
Figure 4-9. Snapshot of the simulated (a, b) temperature and (c, d) vorticity scaled by Coriolis parameter at 100 m after reaching dynamic quasi-equilibrium in the reentrant channel. Panel (a) and (c) are for the 2nd-order TVD scheme; (b) and (d) are for the 3rd-order WENO scheme.

4.4 Preliminary application on the Gulf Stream

Circulation patterns on the MAB continental shelf are driven by large-scale processes. The equatorward shelf current is the strongest signal on the inner shelf, while the poleward flowing the Gulf Stream is dominant near the shelf break in the upper ~200 m. The Gulf Stream path veers towards the open ocean near Cape Hatteras where the current begins to transition from a topographically trapped western boundary current to a vigorously meandering free jet. Recent observations suggest that larger variability of this separation points may be a plausible cause for the warming of the MAB and local relative sea-level rise (Andres, 2016; Ezer, 2013). This baroclinic instability creates complex eddies and counter-currents between the Gulf Stream and the shelf currents (Chen et al., 2014a). The variability in location, shelf intrusion, meandering,
and eddy shedding associated with the Gulf Stream and their implications on near-shore processes are active research topics in the ocean modeling community.

So far, most of the modeling efforts are based on SG models (e.g., Zeng and He, 2016), where bathymetry smoothing at large slopes and grid nesting in coastal regions are often required. On the other hand, a successful application of an UG model to this system can enable new research topics on cross-scale processes such as shelf-ocean exchanges and canyon processes. However, it should be noted the results presented here are preliminary and mainly for the qualitative comparison between the new and old schemes. A comprehensive assessment on model skill is ongoing.

The model domain covers the north-west Atlantic, the Gulf of Mexico, and the Caribbean Sea (Figure 4-10). The horizontal grid has 388K nodes and 766K elements, with a resolution of ~7 km in the open ocean, smoothly transitioned to ~2 km near the coastline. The vertical grid uses the terrain following LSC^2 coordinate (Zhang et al., 2015) with variable numbers of layers depending on depths (27.0 layers on average). Applied at surface are atmospheric forcings from NARR, including air temperature, surface pressure, humidity, wind speed and direction, short-wave and long-wave radiation. Initialized from HYCOM reanalysis product on April 1, 2012, the model was run for 170 days with a time step of 150 seconds. Since the initial condition is derived from HYCOM, we consider the model properly spun up after 2 weeks (similar to Zeng and He, 2016). However, we also found mismatches in SST and SSH between the initial HYCOM results and observation (not shown) and therefore our model may need a longer spin-up period to ‘forget’ about these initial errors. This can also explain a part of the model error reported below; therefore, the focus here is the relative performance of different schemes. It is worth noting that the model setup differs from other SG models in using: (1) locally refinement (~2 km resolution) near the shoreline and islands; (2) original, non-smoothed bathymetry (Figure 4-10); (3) no data assimilation. To compare with the new WENO
scheme, we also conducted a simulation using the 2\textsuperscript{nd}-order TVD scheme. We focus on the following two aspects in the comparison:

Figure 4-10: Domain and bathymetry of the large-scale model.

(1) The intensity of the simulated relative vorticity, which is a good indicator of the model’s capability in resolving baroclinic instability. Figure 4-11 shows the simulated vorticity in the Atlantic Ocean at the end of the 170-day simulation. The values at 100 m below surface rather than at surface are shown to exclude wind effects. The pattern is largely consistent between the 2\textsuperscript{nd}-order TVD scheme and the 3\textsuperscript{rd}-order WENO scheme, where the Gulf Stream core is identifiable by large positive vorticity and counter-rotating eddies on its flanks. Compared to the relatively smooth features with the lower-order scheme, the new scheme generates more energetic and refined eddying patterns. In fact, the new scheme leads to a \(~20\%\) increase on average in the simulated eddy kinetic energy (Figure 4-12).
(2) The meanders and eddies associated with the Gulf Stream, which have major implications for the exchange of water masses and tracers between ocean, shelf and coastal regions (Ryan et al., 2001). Within the simulation period, such an event occurs in mid-July (about 100 days from the beginning of the simulation). On July 16, three obvious northward meanders have developed in the core as highlighted by the solid ellipsis in Figure 4-13a (left panel). In fact, the Gulf Stream core has already shed a warm eddy toward Gulf of Maine. Within five days (on July 21; Figure 4-13b), the meander in the middle also starts to fold on itself and shows signs of eddy de-attachment. These features are not easily seen in the model results with the old scheme (Figure 4-13ab, middle panels), where the signature of the Gulf Stream becomes too diffused after its separation from Cape Hatteras and any eddy detachment is nearly non-existent. In contrast, the new WENO scheme qualitatively captures this event (Figure 4-13ab, right panels), although the features tend to be exaggerated. The exaggeration is likely due to the over-prediction in SST or the rough representation of the Chesapeake Bay by a point source, and further calibration is warranted.
Figure 4-11: Simulated relative vorticity (scaled by Coriolis parameter) at $z=-100$ m (cut off at shelf break) at the end of the 170-day simulation: (a) 2nd-order TVD; (b) 3rd order WENO.

Figure 4-12: Simulated eddy kinetic energy at $z=-100$ m, averaged over the entire domain.
Figure 4-13: Snapshots of SST showing an eddy-shedding event (black circle): (a) intensive meanders formed; (b) eddies shedding from the meanders.
4.5 Conclusions

In this chapter, a 3rd-order transport scheme based on WENO is designed for improving the skill of our cross-scale UG model in the eddying regime. The specific designs focus on striking a balance among accuracy, monotonicity, efficiency, and robustness. We show that eddies and filaments are better resolved using this new scheme with benchmark tests and a field application to the Gulf Stream. Although not shown here, the new scheme also slightly improves the simulated salinity intrusion and stratification in an estuarine setting.

From the preliminary application to the Gulf Stream, the new 3rd-order scheme seems adequate in resolving major eddying features associated with a strong western boundary current. We note that no explicit diffusion or diffusive filters are applied to control numerical dispersion, which would otherwise degrade order of convergence. Nevertheless, minor over/under-shoots can happen locally in a large gradient zone, since the scheme is “essentially non-oscillatory”, but these are minor enough to be tolerated by the model. A 4th-order scheme could also be constructed by applying the approach of optimal weighting of Liu et al. (2013), although it entails higher computation and communication cost, and may trigger larger numerical dispersion that must be carefully filtered. The 3rd-order scheme seems to resolve the Gulf Stream meanders and eddies well, at a cost of 20-30% more computational time than the TVD scheme.
5 Summary

The main goal of this dissertation is two-fold: the first is to develop numerical methods that improve the cross-scale capability of our unstructured-grid (UG) model in general; the second is to use the newly developed techniques to construct a Chesapeake Bay model that efficiently and accurately handles a domain from the eddying ocean to any sub-tributaries of interest, and to study the interrelated processes on multiple scales in a seamless and holistic fashion.

The development work on numerical schemes tackles two major obstacles in UG coastal and regional modeling, namely the efficiency bottleneck and the lack of skills in the eddying regime. Our main contribution includes two new transport schemes specifically designed for addressing each of the two obstacles in cross-scale applications, thus significantly advancing the state of science of UG based modeling.

The first new transport scheme utilizes an implicit TVD scheme to alleviate the efficiency bottleneck often encountered in large vertical flow over steep slope while maintaining high accuracy. This ensures that true physics are simulated on the original non-smoothed bathymetry with a reasonable computational cost. Moreover, with this development, a model domain with extremely large scale contrasts (> 3 orders of magnitude) becomes attainable for baroclinic simulations, as illustrated by the examples shown in Chapter 2 and 3, as well as our on-going marsh migration study and an engineering study presented in Liu et al. (submitted). Of course, the characteristic temporal scale of the processes must also be resolved by the model time step; this is not an issue because the typical time step of a baroclinic simulation is around 100-300 seconds, which is smaller than typical scales as found in tidal and tracer transport processes (and the scales are even larger in the eddying regime). Efficient baroclinic simulations with
local refinements are also a highly desirable capability for management who often practices in small-scale local systems that are tightly linked to large-scale remote processes.

The second new transport scheme uses a 3rd-order horizontal transport scheme based on WENO formulation in order to improve the model skills in the eddying regime, which is a major challenge for UG models (Danilov, 2013). The eddy-resolving capability provided by the new scheme allows the integration of meso-scale processes and small-scale coastal processes in a holistic baroclinic model, which opens up new opportunities to close the current knowledge gaps in the study of estuary-ocean interaction and canyon processes.

We have applied the newly developed methods to our main test bed of Chesapeake Bay. A seamless cross-scale model based on SCHISM is built from sub-tributaries into the eddying regime. While this work is still on-going, we have already achieved significant advances in capturing key processes from a wide range of spatial scales, e.g., coastal upwelling, salinity intrusion and the associated channel-shoal contrast, the unique three-layer circulation in a tributary (Baltimore Harbor) etc. More importantly, these are achieved with a faithful representation of the underlying bathymetry, which is critical in reducing artificial biases in the estimates of important variables, such as hypoxic volume, plume extent, and bottom stress. The Bay SCHISM model facilitates the quantitative analyses on mechanism and processes that are otherwise difficult to quantify. The model has also been successfully applied in several inter-disciplinary studies (e.g., the phytoplankton dynamics by Wang (2017)), as well as assisting decision makers in assessing the effects of the proposed engineering projects on local hydrodynamics and water quality (Ye et al., submitted; Liu et al submitted; Zhang and Wang, 2016).

For future research, some applications that can immediately benefit from the new numerical techniques and the Bay model developed in this dissertation are discussed as follows:
(1) With the efficiency bottleneck alleviated in Chapter 2, small-scale processes that are unique in shallow regions and tributaries can be simulated with affordable computational cost. One potentially interesting process is the small-scale eddies induced by irregular channel geometries in tributaries. In these areas, the velocity is generally small and the eddies may play an important role on local residence time. The representation of such small-scale processes needs locally high resolution, which is now feasible.

(2) Although not discussed in detail in Chapter 3, the signals of coastal upwelling events are indeed captured by the SCHISM Bay model. By tracking the movement of the bottom cold water, it is clearly seen that the intrusion into the Bay is enhanced during the upwelling events. Quantifying the effect of wind on intrusion length/pathway into the Bay and exploring the implications on water quality and biological processes have already produced promising results (Wang, 2017), and other applications (e.g. fishery) will also be pursued.

(3) With the new WENO scheme showing improved model skill in the eddying regime, the next step would be a comprehensive model calibration and assessment on the large-to-small domain including the Gulf Stream. This would be a powerful model for studying the flow over steep shelf slope, canyon dynamics, internal waves, and estuary-shelf-ocean exchanges of water masses and tracers.
Literature Cited


Cerco, C., Kim, S.C. and Noel, M., 2010. The 2010 Chesapeake Bay Eutrophication Model. A Report to the US Environmental Protection Agency Chesapeake Bay Program and to the US Army Engineer Baltimore District. US Army Engineer Research and Development Center, Vicksburg, MS.


Appendices

Appendix A: Additional model-data comparison for the SCHISM Bay model
Salinity profiles on selective stations both in the main channel (a-e) and on the shoal (f-g).
Figure A1: Selective salinity profile comparisons at main channel stations: (a) CB7.4, (b) CB7.1S, (c) CB4.4, (d) CB3.3C, (e) CB3.1; and shoal stations: (f) CB6.3, (g) CB4.3E, (h) CB3.3E.
Temperature time series

![Temperature time series graphs for various depths and locations showing temperature changes over time.](image-url)
Figure A2: Temperature time series for 2011-4 at main stem stations. For the simulated bottom values, the shaded regions correspond to the ranges of the bottom observation depths, which vary through time.
Figure A3: Comparison of monthly SSC in 2012 from (a) HF radar (the red arrows show the averaged wind direction and the number is the averaged wind magnitude); (b) SCHISM (wind direction arrows are omitted). The HF radar data start in July 2012.
Figure A4: comparison of surface current on June 9, 2013 among (a) HR radar, (b) SCHISM and (c) HYCOM.
VITA

Fei Ye was born in Changchun, China on 3 May 1985. He earned a Bachelor degree in Environmental Engineering emphasizing on water resources and water treatment technology from Hohai University, Nanjing, China. In 2007, he entered the M.S. program in Ecology focusing on riparian ecosystems at the Research Center for Eco-Environmental Sciences, Chinese Academy of Sciences under the guidance of Dr. Qiuwen Chen, then bypassed to a doctoral program focusing on riparian vegetation dynamics under reservoir operations, and earned a Ph.D. degree in Environmental Engineering (different from the M.S. program due to the interdisciplinary nature of the research) in 2012. During the same period, he worked as a research assistant in the “State Key Laboratory of Urban and Regional Ecology” and the “State Key Laboratory of Environmental Aquatic Chemistry” in the same institute. After a one-year stay at VIMS as a visiting scientist in 2012, he decided to enter the current Ph.D. program in 2013 under the guidance of Dr. Joseph Zhang. He will graduate in January, 2018.