

Third-order WENO transport scheme for simulating the baroclinic eddying ocean on an unstructured grid

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ABSTRACT

Despite the recent success achieved by the unstructured-grid SCHISM (Semi-implicit Cross-scale Hydroscience Integrated System Model) in multi-resolution studies, its skill in simulating the baroclinic eddying ocean needs to be further improved. In particular, the classical 2nd-order transport schemes for estuaries and coastal zones are too dissipative to resolve the baroclinic dynamics associated with strong boundary currents, such as meso-scale meanders and eddies. To close this gap, this paper presents a newly designed 3rd-order finite volume transport scheme, based on the Weighted Essentially Non-Oscillatory (WENO) formalism. This new scheme strikes a delicate balance among accuracy, efficiency, and monotonicity for the transport in the eddying regime. Idealized numerical benchmark experiments demonstrate that the WENO scheme is very effective in limiting numerical diffusion. The scheme is then applied in a realistic simulation of the Gulf Stream and the surrounding circulation, further confirming its capability of resolving baroclinic meso-scale eddies and meanders. This new high-order transport scheme is therefore ideal for extending the ability of SCHISM to study cross-scale baroclinic applications that range from the river dynamics to the eddying ocean processes.

1. Introduction

The past two decades have seen wider adoption of unstructured-grid (UG) models in coastal ocean modeling, mainly due to UG's flexibility in (1) resolving bathymetric and geometric features, and (2) local refinement/de-refinement for the area of interest/disinterest. A key remaining challenge for UG model development is to fully realize its potentials in cross-scale baroclinic problems. A review by Danilov (2013) indicates that until recently large-scale ocean applications are still lacking in the UG model community. *Baroclinic* applications of UG models had been mostly confined to coastal regions (Chen et al., 2003; Fringer et al., 2006; Zhang and Baptista, 2008) and rarely extended to the eddying ocean; a recent effort in allowing eddy-resolving capability in a coastal UG model (Thetis) was presented by Kärnä et al. (2017), but realistic applications are still lacking. Recently, a good 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/resolving capability. Different from the coastal models, the designs of these UG models aim at simulating the global ocean circulation rather than finer-scale coastal processes. One example of such designs is the Spherical Centroidal

Voronoi Tessellations used in MPAS-Ocean (Ringler et al., 2013), which handle multi-resolutions well for the more regularly shaped deep ocean. However, this design is still not cost-effective in resolving highly irregular geometries in estuaries and coastal regions, so a coupling with a UG coastal model is often required to relate global/basin scale ocean processes to local estuarine/coastal processes.

The gap between global UG models and coastal UG models 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 reduces the size of the computational grid, but more importantly also 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 (Ye et al., 2018), we observed errors that most likely came from the ocean boundary conditions derived from the global HYCOM reanalysis product.¹ 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 felt.

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¹ Url: <https://www.HYCOM.org/dataserver/gofs-3pt0/reanalysis>, last accessed Jan 1, 2019.

The goal of this study is to enhance UG coastal models' capability in resolving the baroclinic circulation in the open ocean eddying regime, with the numerical implementation done in SCHISM (Semi-implicit Cross-scale Hydrosceince Integrated System Model; schism.wiki). Previously, high-order *momentum* advection schemes that use viscosity/filters as stability function have been developed in SCHISM by Zhang et al. (2016) to address the issue of spurious modes (exhibiting as noises in the velocity fields). For recent applications in the eddying regime (e.g., Yu et al., 2017), the high-order *momentum* schemes were used along with a 2nd-order tracer *transport* scheme. Although the latter's numerical dissipation is considered sufficiently small for estuarine applications, we find its utility in simulating meso-scale eddies and meanders is still less than satisfactory. This is likely because the intrinsic physical dissipation is large in estuaries due to bottom friction and irregular geometry/bathymetry, which may effectively mask numerical dissipations. In an eddying ocean, however, the forces are largely balanced (Ringler et al., 2013) and physical dissipation is at a much lower level. Therefore, the numerical dissipation needs to be carefully controlled and higher-order transport schemes are generally deemed necessary in the eddying regime.

To improve SCHISM's capability in the eddying ocean, we seek a transport scheme that is (1) easily extendable to 3rd or higher order accuracy; (2) monotonic or nearly so; (3) robust and efficient on generic unstructured grid (without geometric constraints, such as orthogonality or mesh quality). For the first requirement on accuracy, our recent applications on Kuroshio Currents (Yu et al., 2017) showed that the existing 2nd-order transport scheme only needs modest improvement, so a third-order scheme is preferred over a fourth-order scheme because the former's leading truncation errors are in the form of diffusion instead of dispersion, greatly reducing the need for applying additional explicit diffusion to avoid unphysical oscillation (Hirsch, 2007). The second requirement on monotonicity is necessitated by the large spatial gradients in dissolved substances' concentrations in nearshore regions or across the base of the mixed layer in the deep ocean, which may trigger unwanted numerical oscillations. Although various filtering techniques have been proposed before (Shchepetkin and McWilliams, 2005), they are not ideal because they reduce the effective order of accuracy. The third requirement on robustness and efficiency is mainly to accommodate cross-scale applications, which are characterized by transitions from coarser and relatively uniform meshes in the ocean to finer and relatively irregular meshes in coastal regions. Previously, the performance of various advective schemes for UG ocean modeling have been summarized by Hanert et al. (2004) and Budgell et al. (2007). The latter showed that the computational cost can increase significantly with the requirement of higher-order accuracy and the techniques for limiting numerical oscillations. For our purpose of improving SCHISM's eddy-resolving capability, only a modest improvement on horizontal advection accuracy would be required. But we do need a scheme design that is flexible enough to balance between accuracy and other above-mentioned requirements, especially the computational cost, for which purpose the WENO scheme serves as a good candidate or compromise (Long et al., 2008). Introduced by Liu et al. (1994), the WENO scheme has been applied in various fields including computational fluid dynamics, astrophysics, and biology; the review by Shu (2009) provides a comprehensive list of the related applications. In the field of ocean modeling, it has been adopted by the structured-grid (SG) model ROMS on sediment transport in the vertical dimension (Warner et al., 2008). After the extension to UGs (Friedrich, 1998; Hu and Shu, 1999), WENO has also attracted attention in the field of morphodynamics (Canestrelli et al., 2010; Guérin et al., 2016). To our knowledge, WENO has not been applied to the horizontal tracer transport in UG models.

In this paper, we present a numerical scheme based on WENO formalism for the horizontal transport in the UG modeling system SCHISM, aiming at better resolving meso-scale eddies and meanders in the eddying regime. The following text is structured as follows: Section 2 briefly introduces the discretization of transport equation in SCHISM, then explains the challenges of adapting WENO in SCHISM and how we design

the finite volume solver accordingly. Section 3 presents the results from a numerical benchmark, confirming the superior behavior of the new scheme compared to lower-order schemes (2nd-order schemes are commonly used for the estuarine tracer transport in coastal models). Section 4 applies the new scheme to simulate the Gulf Stream and its surrounding circulation, then compares the performance between the new scheme and a classical 2nd-order TVD scheme (see details in Section 3.1 of Zhang et al. (2016)), followed by the conclusions in Section 5.

2. Methods

Since the focus of this study is the transport solver, we will not repeat all governing equations in SCHISM, for which readers are referred to Zhang et al. (2016). The transport equation and its discretization in SCHISM are described below to provide a background.

2.1. Transport equation and operator splitting

The transport equation solved by SCHISM reads:

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

where T is the concentration of a generic tracer; κ is vertical eddy diffusivity ($\text{m}^2 \text{s}^{-1}$); q includes all source and sink terms; $\mathbf{u}$ is the three-dimensional velocity vector (u, v, w) (m s^{-1}). We have neglected horizontal diffusion in Eq. (1) for brevity, as its implementation is straightforward (Zhang and Baptista, 2008). In a finite volume framework (Fig. 1), the discretized form of Eq. (1) that centers on Prism i is expressed as:

$$T_i^{n+1} - T_i^n = -\frac{\Delta t}{V_i} \left\{ \sum_{j \in S_i} [Q_j(T_j' - T_i)] \right\} + \frac{A_i \Delta t}{V_i} \left[\left(\kappa_j' \frac{\partial T_j}{\partial z} \right)_{j=i \cap i^+} - \left(\kappa_j' \frac{\partial T_j}{\partial z} \right)_{j=i \cap i^-} \right] + \frac{\Delta t}{V_i} \int_{V_i} q dV, \quad (2)$$

where i is the prism index; j is the face index; n is the time level. T_i is the average concentration of Prism i defined at prism centers. V_i is the volume of Prism i . S_i denotes all faces of Prism i ; Q_j is the total volumetric flux through Face j (positive going outward Prism i), which is already known after solving the momentum equation at the current step. T_j' is the average concentration over Face j , such that the mass flux through Face j can be expressed as $Q_j T_j'$. For the diffusion term, i.e. the 2nd term on the right-hand side (RHS) of Eq. (2), additional symbols are introduced for convenience (Fig. 1b): 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 . κ_j' is vertical diffusivity defined at top and bottom faces of a prism. A_i is the projected area of prism i onto the horizontal plane. The time levels of T on the RHS will be specified next.

SCHISM applies an operator splitting procedure in solving the transport equation (Zhang et al., 2016). Based on the discretized transport equation (2), T_i^n is advanced to T_i^{n+1} in three steps: horizontal advection, vertical advection, and vertical diffusion plus other terms. Each step deals with different terms on the RHS of Eq. (2):

Step 1 horizontal advection

$$T_i^{(1)} - T_i^n = -\frac{\Delta t}{V_i} \left\{ \sum_{j \in S_i^H} [Q_j(T_j' - T_i)] \right\}, \quad (3)$$

Step 2 vertical advection

$$T_i^{(2)} - T_i^{(1)} = -\frac{\Delta t}{V_i} \left\{ \sum_{j \in S_i^V} [Q_j(T_j' - T_i)] \right\}, \quad (4)$$

Step 3 vertical diffusion and source

$$T_i^{n+1} - T_i^{(2)} = \frac{A_i \Delta t}{V_i} \left[\left(\kappa_j' \frac{\partial T_j}{\partial z} \right)_{j=i \cap i^+}^{n+1} - \left(\kappa_j' \frac{\partial T_j}{\partial z} \right)_{j=i \cap i^-}^{n+1} \right] + \frac{\Delta t}{V_i} \int_{V_i} q dV, \quad (5)$$

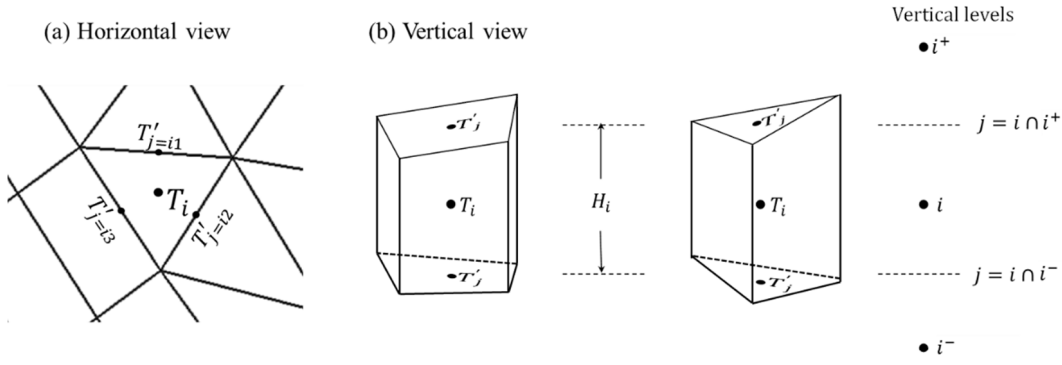


Fig. 1. The finite volume framework for SCHISM's transport solver: (a) horizontal view; (b) 3-D view of two types of control volumes. In SCHISM, the tracer concentrations (T) are defined at prism centers; while the average face concentrations (T') need to be reconstructed.

where S_i^H denotes the faces of Prism i that are parallel to the z -coordinate; S_i^V denotes the top face ($i \cap i^+$) and the bottom face ($i \cap i^-$) of Prism i , which may or may not be parallel to the horizontal plane (Fig. 1b). For the horizontal advection, a 2nd-order TVD scheme is sufficient for estuarine applications (Zhang et al., 2016; Ye et al., 2018), but not for the eddying ocean (Section 4.3); so the main task here is to find a better approximation for the average interface value T'_j in Eq. (3). This step is treated explicitly because horizontal advection is generally not the bottleneck for efficiency. Since Eq. (3) is an explicit scheme, its time step is limited by:

$$\Delta t \leq \frac{V_i}{\left| \sum_{j \in S_i^{H+}} Q_j \right|} C, \quad (6)$$

where S_i^{H+} is a subset of S_i^H , denoting the faces with *outflowing* fluxes. The CFL condition for WENO schemes is typically $C = 0.6$ - 0.8 (Zhou et al., 2001) and a smaller value ($C = 0.4$ - 0.6) is often used for solutions with discontinuity (Titarev and Toro, 2005). Here, a default value of 0.5 is chosen, which is adjustable as a parameter in SCHISM. For the vertical advection, an implicit 2nd-order TVD scheme was previously designed for SCHISM (Zhang et al., 2016) to avoid small time steps and maintain accuracy. We have not applied higher-order schemes for Step 2 and Step 3, because the grid spacing in the vertical dimension is typically much smaller than that in the horizontal dimension. Our previous applications showed that 2nd-order accuracy is sufficient to resolve sharp pycnocline in non-eddying regimes (Ye et al., 2016, 2018). Early applications of SCHISM in the eddying regime (Section 4) show that the skill in capturing vertical temperature gradient is similar to the data-assimilated HYCOM, but more challenging applications (e.g., on submarine canyon processes) are needed to further assess the vertical transport scheme.

2.2. Transport solver design

The existing WENO schemes on UG mainly comprise of two types (Liu and Zhang, 2013), with Type I focusing on non-linear stability and Type-II focusing on achieving higher-order accuracy. The scheme designed in this section belongs to Type I. Compared to existing schemes, we put more emphasize on simplifying the stencil to balance between the desired accuracy and efficiency/robustness, so that the scheme is suitable for *cross-scale* estuarine/ocean *baroclinic* applications on *generic* UGs carried out by *parallel* machines. For this purpose, the following specific considerations were taken into account in the design: (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 WENO procedure described below.

2.2.1. Numerical flux and stencils

A key step in the WENO procedure is to reconstruct the interfacial mass flux, namely the term $Q_j T'_j$ in the discretized horizontal advection equation (3). Following Hu and Shu (1999), a q -point Gaussian integration is used:

$$Q_j T'_j \approx \sum_{k=1}^q Q_j \xi_k T'(x^{G_k}, y^{G_k}), \quad (7)$$

where $Q_j T'_j$ is the mass flux through Face j ; (x^{G_k}, y^{G_k}) are the global coordinates of the k th quadrature point on Face j , with ξ_k as its weight. In SCHISM, tracer concentration is treated as vertically homogeneous within each prism (Zhang et al., 2016), so we only need to decide the locations of quadrature points on each side in the horizontal dimension. Since Gaussian integration is precise for polynomials of degree $(2q-1)$ or less, $q = 1$ (one point at the side center) and $\xi_1 = 1$ are chosen when linear polynomials are needed; whereas $q = 2$ (two points on each side with distances of $\pm \frac{l}{2\sqrt{3}}$ from the side center, where l is the side length) and $\xi_1 = \xi_2 = 0.5$ are chosen when quadratic polynomials are needed (Hu and Shu, 1999). The use of Gauss-Legendre quadrature rule with all positive weights does not introduce stability problem (Huybrechts, 2009). The subscript k is dropped in the subsequent description, because the reconstruction procedure is identical for each quadrature point. Note that the interfacial volume flux Q_j can be taken out of the summation on the R.H.S. of Eq. (7), because it is independent of tracer concentration and treated as a constant on Face j . For simplicity and efficiency, the upwind flux is used, i.e. the face value is only reconstructed with stencils centered on the upwind prism (Fig. 2). This seems sufficient for our applications in the eddying ocean (e.g., the test case in Section 4). Other numerical fluxes have been applied for WENO schemes (Titarev and Toro, 2005); assessing the cost-effectiveness of different numerical fluxes for ocean transport are left for future studies.

The next step is to reconstruct the face value $T'(x^G, y^G)$ in Eq. (7) by prismatic values. This is illustrated by a sample horizontal mesh in Fig. 2. In this horizontal view, we will use “elements” instead of “prisms” to avoid confusion. Based on an appropriate choice of stencil, a polynomial of degree n (denoted as “ p^n ”) can be constructed. Since we are using the upwind flux, these stencils are centered on the upwind element of (x^G, y^G) . Specifically, we look for stencils associated with the “Tier-1 neighborhood”, which is defined by the elements that share 1 or 2 nodes with the center element (Fig. 2). Starting from the center element, the stencil candidates are constructed by sequentially listing the elements in this neighborhood in counter-clockwise order. Both 2nd-order and 3rd-order reconstructions are discussed next.

A 2nd-order reconstruction requires a linear polynomial, which can be expressed as:

$$p_s^1 = [1 \ x \ y] \begin{bmatrix} a_s \\ b_s \\ c_s \end{bmatrix} \equiv \mathbf{LC}, \quad (8)$$

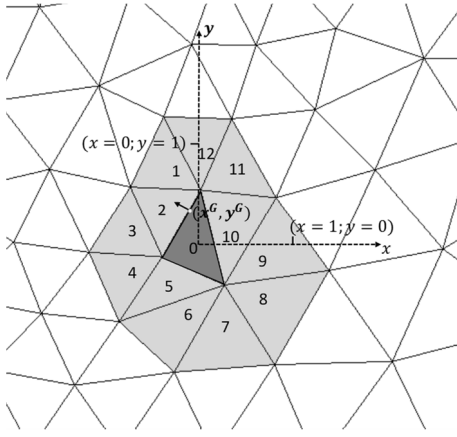


Fig. 2. The neighborhood (gray) for selecting WENO stencils centered at Element 0. For example, for the side marked by the black arrow (denoting velocity direction), a stencil can be constructed by its upwind element ‘0’ plus two (for linear stencils) or five (for quadratic stencils) neighboring elements. A local coordinate is used for each stencil (dashed lines), with the origin on Element 0’s centroid, and the coordinates normalized by the distance between the origin and the centroid of the furthest neighboring element (Element 8 in this case).

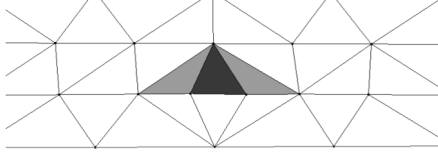


Fig. 3. An invalid stencil for constructing a linear polynomial; the centroids of the three elements are co-linear.

where s is the stencil index among all possible stencils centered on the upwind element of (x^G, y^G) ; $\mathbf{C} \equiv [a_s b_s c_s]^T$ is a group of coefficients to be determined by the information from the elements within Stencil s . In this case, three elements are needed; for example, the potential choices in Fig. 2 are 0–1–2, 0–2–3, ..., 0–12–1. Inserting the concentration values and coordinates from the three elements of Stencil s into Eq. (8), we have:

$$\mathbf{T} \equiv T_k = [1 x_k y_k]_{3 \times 3} \begin{bmatrix} a_s \\ b_s \\ c_s \end{bmatrix}_{3 \times 1} \equiv \hat{\mathbf{L}} \mathbf{C}, \quad (9)$$

where $k = 1, 2, 3$ is the local element index within Stencil s ; $\mathbf{T} \equiv T_k$ is the concentration values at element centers. The polynomial’s coefficients $\mathbf{C} \equiv [a_s b_s c_s]^T$ are found by $\mathbf{C} = \hat{\mathbf{L}}^{-1} \mathbf{T}$.

Similarly, a 3rd-order reconstruction requires a quadratic polynomial:

$$p_s^2 = [1 \ x \ y \ x^2 \ xy \ y^2] \begin{bmatrix} a_s \\ b_s \\ c_s \\ d_s \\ e_s \\ f_s \end{bmatrix} \equiv \mathbf{L} \mathbf{C}. \quad (10)$$

In this case, 6 elements are needed, which are also chosen from “Tier-1”; for example, the potential choices in Fig. 2 are: 0-1-2-3-4-5, 0-2-3-4-5-6, ..., 0-12-1-2-3-4. The procedure of finding the coefficients $\mathbf{C} \equiv [a_s b_s c_s d_s e_s f_s]^T$ is similar to that in the linear case, which will not be repeated.

Tier-1 neighborhood is chosen because: (1) it generally allows quadratic polynomials that lead to 3rd-order accuracy on a triangular mesh; (2) it simplifies the MPI communication among the neighboring sub-domains; (3) our experience suggests that Tier-1 stencils are generally less prone to oscillations than Tier-2 stencils (center element

+ “Tier-1 neighbors” + “Tier-1 neighbors of neighbors”). To reduce truncation error, normalized local coordinates are used within each big stencil (Element 0 and other gray elements in Fig. 2), such that: (1) the coordinate origin coincides with the centroid of the center element; (2) the x and y axes are scaled (without rotation) by the distance between the origin and the furthest neighbor’s centroid. Then, the value at each quadrature point is reconstructed by a linear combination of the polynomials from all stencils:

$$T'(x^G, y^G) = \sum_{s=1}^{N_s} w_s p_s^n(x^G, y^G), \quad (11)$$

where s is the stencil index; N_s is the total number of stencils; w_s is the linear weight of each stencil, which is to be determined later; p_s^n is a polynomial of degree n based on the s th stencil. The polynomials (p_s^n) in Eq. (11) are exact at element centers and $(n+1)$ th order accurate elsewhere; moreover, it is possible to achieve $(n+2)$ th order accuracy through an optimal choice of the weighting w_s (Hu and Shu, 1999).

2.2.2. Weights

Although higher-order accuracy can be achieved by weight optimization (Hu and Shu, 1999), we choose not to do so. The rationale is that 3rd-order accuracy is sufficient for our present applications; more importantly, optimal weighting is not always guaranteed on a generic UG (with abrupt element size transitions and skew elements), which reduces the robustness of the algorithm in cross-scale applications. We may adopt optimal weighting if there is a need for 4th-order accuracy in future applications. Currently, w_s is solely determined by the concentration gradient within each stencil (following Hu and Shu (1999), but without optimal weighting):

$$w_s = \frac{\hat{w}_s}{\sum_{s'=1}^{N_s} \hat{w}_{s'}}, \text{ with } \hat{w}_{s'} = \frac{1}{(\epsilon + [IS]_{s'})^2}, \quad (12)$$

where ϵ 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 negligible violations in monotonicity, whereas $\epsilon > 10^{-4}$ tends to generate noticeable oscillations near large tracer gradients; $[IS]$ is a smoothness indicator following Hu and Shu (1999)’s formulation. For linear stencils leading to a 2nd-order reconstruction, the smoothness indicator is:

$$[IS]_s = \frac{1}{A} \int \left[\left(\frac{\partial p_s^1}{\partial x} \right)^2 + \left(\frac{\partial p_s^1}{\partial y} \right)^2 \right] dS, \quad (13)$$

where p_s^1 is a linear polynomial based on the s th stencil, A is the area of the centering element, $\int dS$ is an integration over the area of the centering element. For quadratic stencils leading to a 3rd-order reconstruction, the smoothness indicator is:

$$[IS]_s = \frac{1}{A} \int \left[\left(\frac{\partial p_s^2}{\partial x} \right)^2 + \left(\frac{\partial p_s^2}{\partial y} \right)^2 \right] dS + \int \left[\left(\frac{\partial^2 p_s^2}{\partial x^2} \right)^2 + \left(\frac{\partial^2 p_s^2}{\partial x \partial y} \right)^2 + \left(\frac{\partial^2 p_s^2}{\partial y^2} \right)^2 \right] dS, \quad (14)$$

where p_s^2 is a quadratic polynomial based on the s th stencil. In realistic applications of SCHISM, the 3rd-order reconstruction based on quadratic polynomials is applied by default, which occasionally downgrades to the 2nd-order reconstruction in abnormal cases.

2.2.3. Abnormal cases

The use of a generic unstructured grid and a small neighborhood for reconstruction can lead to abnormal cases, which must be carefully handled to ensure robustness. One abnormal case is related to the availability of linear/quadratic polynomials. Fig. 3 illustrates an invalid stencil for constructing a linear polynomial (2nd-order reconstruction), where the three element-centroids are co-linear, causing a singularity

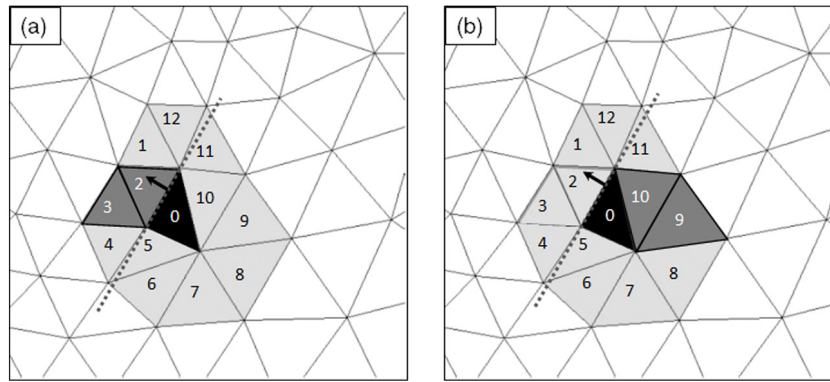


Fig. 4. Linear stencils (dark gray and black elements) centered on Element 0: (a) a stencil with element centroids on both sides of Face 0–2 (including the dashed line), i.e., a straddling stencil for Face 0–2; (b) a stencil with all its element centroids on one side of Face 0–2.

in the matrix inversion associated with the linear reconstruction. A nearly singular stencil can be identified through the condition number of its associated matrix ($\hat{\mathbf{L}}$ in Eq. (9)) while solving for the polynomial coefficients. In our case, since the stencils are already in normalized local coordinates, we simply compute the determinant of the matrix, then remove the stencils with the normalized determinants smaller than a prescribed threshold. A threshold value of 10^{-3} is chosen and sensitivity tests suggest that the results are not very sensitive to this parameter.

Another abnormal case occurs when the so-called “straddling stencils” are the only choices for reconstruction. Fig. 4 shows an example of straddling stencils vs. non-straddling stencils, where Element 2 is downwind of Element 0 and we seek the reconstruction at Face 0–2 (interface between Element 0 and Element 2). Some stencil candidates have elements lying on both sides of that face (e.g., Stencil 0–2–3 in Fig. 4a), which may induce numerical oscillations if there is a shock at Face 0–2. The WENO procedure would assign a small weight to the shock-containing stencil according to Eq. (12); while other stencils not containing the shock (e.g., Stencil 0–9–10 in Fig. 4b) would receive larger weights. Therefore, having stencils from different sectors that covers all directions from the centering element is ideal to prevent oscillations (Hu and Shu, 1999; Liu and Zhang, 2013). However, this may not always be possible for generic UGs, especially when a small neighborhood is used. For example, the number of available choices for 3rd-order stencils is limited on a uniform quadrangle mesh (Fig. 5). In this case, for any given side of Element 0, the candidate stencils are either straddling it (Fig. 5a shows two examples) or singular (Fig. 5b). As a result, excessive numerical dispersion is unavoidable when large concentration gradient is present at the side of interest, because all available (non-singular) stencils would be given similar weights by Eq. (12) even if their $|IS|$ s are all large. A straightforward remedy taken by us is to fall back to 2nd-order stencils, which only require 3 elements and so more stencil choices are available; for example, the 2nd-order stencil 0–1–2 in Fig. 5b is of better quality than the 3rd-order stencil 0–1–2–6–7–8 in suppressing numerical dispersion. The degradation of accuracy from 3rd-order to 2nd-order is not against our objective of improving the model skill in the eddying regime, because triangles are typically used in the open ocean, whereas quadrangles are mostly used to resolve channels inside estuaries (non-eddying regime) where 2nd-order accuracy is sufficient. Alternatively, Tier-2 neighborhood can be used for quadrangular elements to obtain 3rd-order accuracy, but we have not seen its need for now.

The availability of 3rd-order reconstruction in realistic applications is illustrated by two meshes: a Northeast Pacific Ocean mesh with refined Columbia River (Fig. 6a) and a Northwest Atlantic mesh with refined Chesapeake Bay (Fig. 6b). In both meshes, triangles are used in the oceanic region, where stencils for 3rd-order reconstruction are almost always available. The main difference between the two meshes lies inside the *non-eddying* regime, namely Columbia River in Fig. 6a

and Chesapeake Bay in Fig. 6b. The former applies pure triangles throughout the river; whereas the latter applies quadrangles (similar to those in a structured grid) in the deep channels of the bay. As a result, the transport calculation in the Chesapeake Bay channels are mostly 2nd-order accurate (green color in Fig. 6b). Previously, a SCHISM model using a 2nd-order TVD transport scheme was shown to achieve very good skills on salt intrusion and stratification inside the Chesapeake Bay (Ye et al., 2018), so the degradation from 3rd-order to 2nd-order accuracy in the *non-eddying* regime is acceptable there.

2.2.4. Boundary treatments

As illustrated in Fig. 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 (refer to the terms enclosed by “[]” in Eq. (3)). This also applies to the “land boundary” in deeper layers. Take for example the LSC² vertical coordinate (Zhang et al., 2015) used by SCHISM (cf. Section 4.2 and Fig. 10d), the deeper layers touch the land at “degeneration points” where no horizontal flux can go through, since the face area degenerates to 0. 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; the time scale of the relaxation is taken to be around 1 day in realistic applications. The outflow sides take the values from the upwind prisms. For near-boundary sides, 2nd-order accuracy or less is applied since a higher-order accuracy stencil is generally not available due to geometric constraints.

3. Numerical benchmark

3.1. Rotating cone

A rotating cone test case (Hubbard, 1999) was conducted to compare the new 3rd-order WENO scheme with other lower-order schemes in SCHISM. The test domain is a circular 2-D disk centering at $(x = 0, y = 0)$, with a radius of 3600 m. The flow field on the disk was specified as:

$$\begin{cases} u = -wy \\ v = wx, \end{cases} \quad (15)$$

where w is the angular velocity set to $2\pi/3000$ (rad s⁻¹), i.e., the flow field is a solid body rotation with a period of 3000 s. The initial concentration is in the form of a radially symmetric Gaussian hill (Fig. 8a) with the maximum concentration at the center (x_0, y_0) :

$$T_0(x, y) = e^{-\frac{(x-x_0)^2 + (y-y_0)^2}{\sigma^2}}, \quad (16)$$

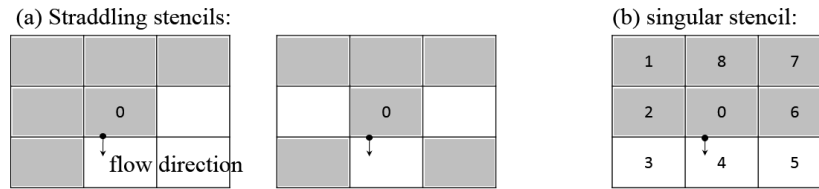


Fig. 5. An abnormal case with a uniform rectangular mesh, where the value on the solid black point is to be reconstructed. Reconstruction based on quadratic polynomials is impossible because all candidate stencils are either straddling the side of interest or singular. Two examples of the straddling stencils are shown in (a) and one example of the singular stencils is shown in (b).

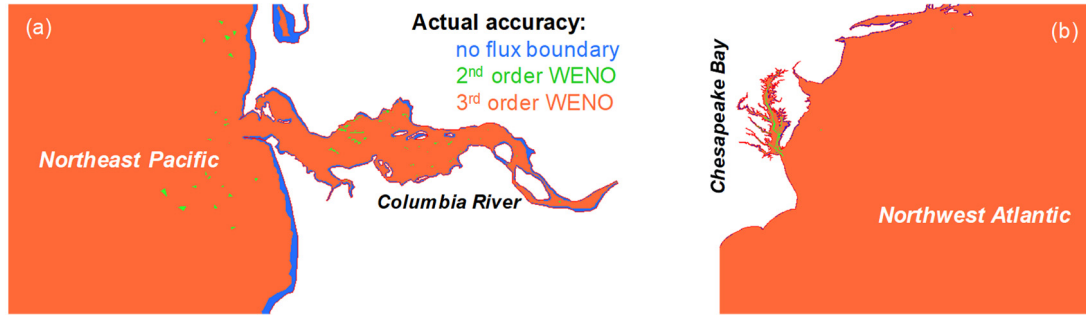


Fig. 6. Availability of 3rd-order accuracy stencils in real applications: (a) US west coast and Columbia River, with a pure triangular mesh; (b) US east coast and Chesapeake Bay, with pure triangles in the ocean and hybrid triangles-quadrangles in the Chesapeake Bay.

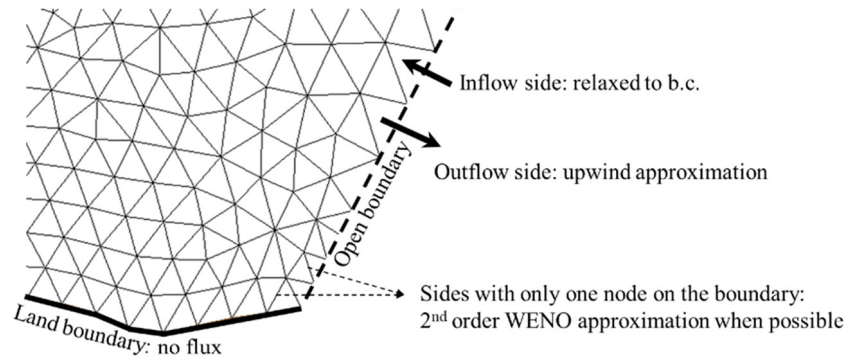


Fig. 7. Boundary treatment for the WENO-based transport in SCHISM.

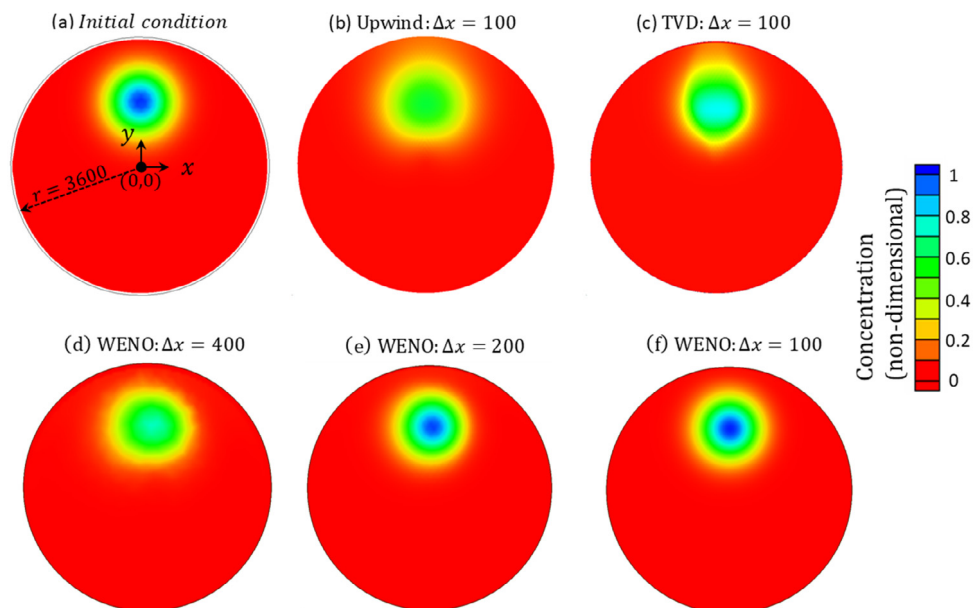


Fig. 8. Rotating cone test showing simulated surface concentration (non-dimensional) of a passive tracer, with model results taken after one rotation from the initial condition: (a) initial concentration; (b) Upwind scheme on a fine mesh; (c) TVD scheme on a fine mesh; (d)–(f) 3rd-order WENO scheme on progressively finer meshes.

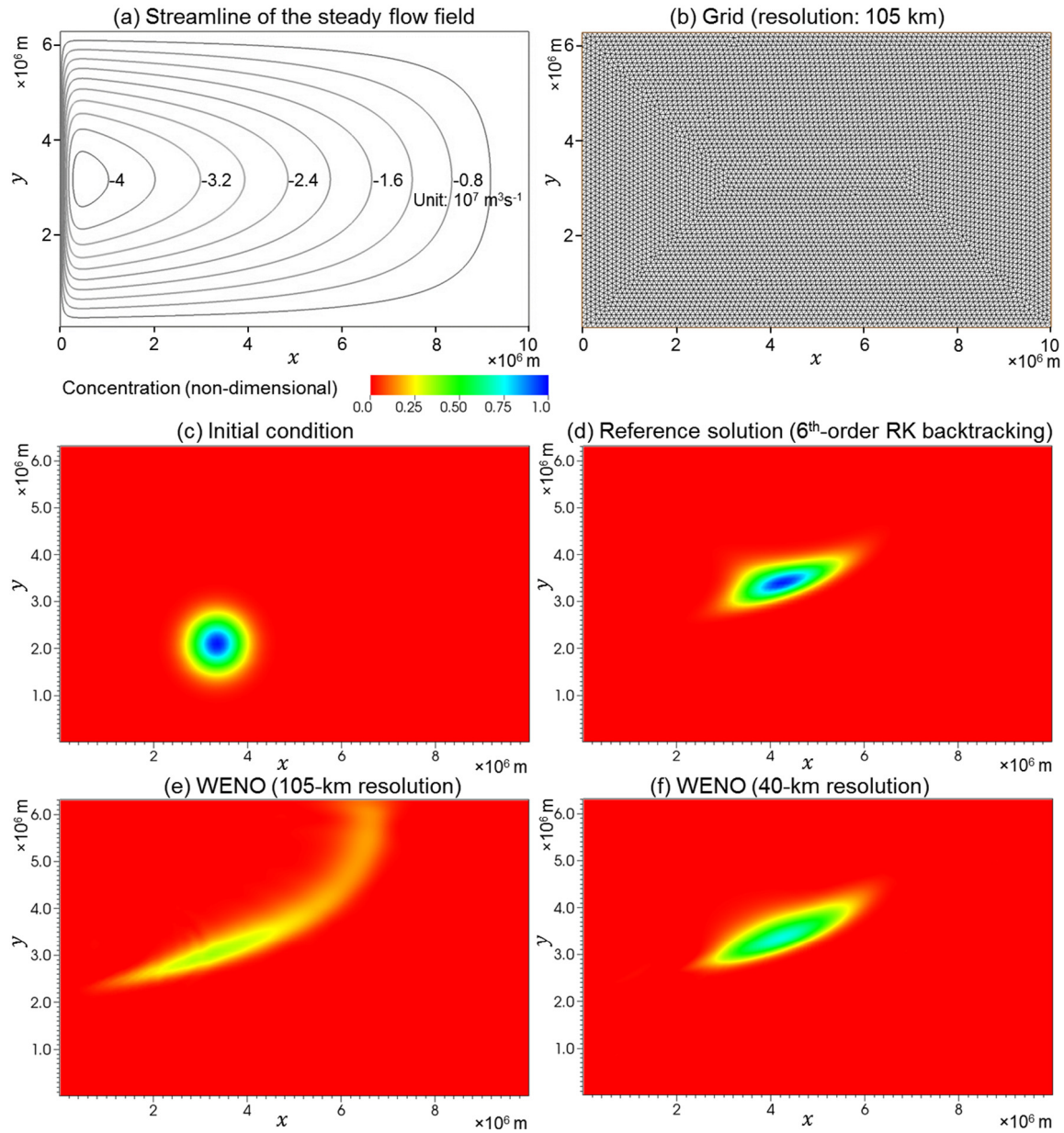


Fig. 9. Advection of a Gaussian hill in the Stommel Gyre. The 40-km resolution grid is omitted because it is similar to the 105-km resolution grid but too dense to show.

where $x_0 = 0$ m, $y_0 = 1800$ m, and $\sigma = 850$ m. The domain was discretized by essentially uniform triangles using DistMesh (Persson and Strang, 2004). The 3rd-order WENO scheme was compared to the 1st-order upwind scheme and the 2nd-order TVD scheme. The maximum Courant number for all tests was chosen as 0.05, representative of the operational value in realistic applications (typically with a horizontal grid resolution of a few kilometers and a time step of a few minutes). After one rotation, the shape of the Gaussian hill was much better preserved by the 3rd-order WENO scheme (Fig. 8ef) than the other two schemes. Even with a low resolution of 400 m (Fig. 8d), the new scheme is comparable to the 1st-order upwind results with a much higher resolution of 100 m (Fig. 8b). The superior performance of the WENO scheme is partly due to its truly multi-dimensional reconstruction; whereas both the upwind and TVD schemes are based on quasi-1D reconstructions (i.e. neglecting the cross-wind direction), hence susceptible to grid orientation. The higher-order accuracy of WENO was achieved at the cost of a 30% increase in computation time compared to the 2nd-order TVD scheme (Table 1). Since WENO is only essentially non-oscillatory, minor oscillations are present in the results.

Table 1

Comparison of different schemes in the rotating cone test with $\Delta x = 100$ m.

	Upwind	TVD	WENO
Root mean square error	0.035	0.017	0.002
Over/under-shoots	0/0	0/0	$0/-2 \times 10^{-5}$
CPU time relative to TVD	0.8	1.0	1.3

In real applications, these are small enough and require no diffusive filters to stabilize.

3.2. Stommel Gyre

The new scheme's performance was further assessed in a test case proposed by Hecht et al. (1995), in which a smooth concentration field was advected by the Stommel Gyre (Stommel, 1948) in a rectangular domain (Fig. 9a). The analytical flow field exhibits westward intensification and large shear, resembling realistic basin-scale wind-driven circulations. The setup here mostly followed that described by Hecht

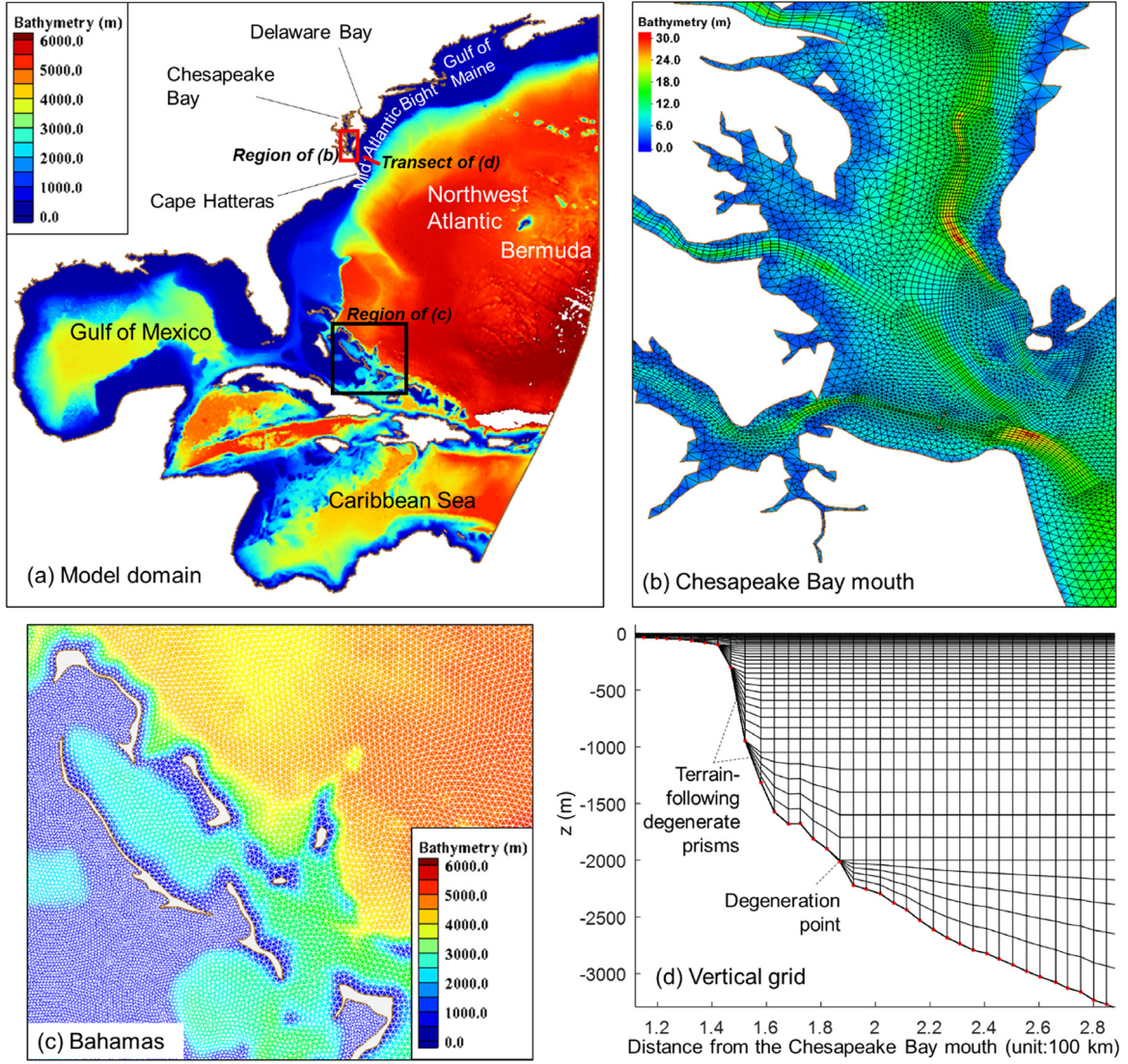


Fig. 10. The regional SCHISM model: (a) domain and bathymetry, with locations of (b)–(d) marked; (b) zoomed-in view on the grid near the Chesapeake Bay mouth, where quadrangles are applied to pave the deep channels; (c) zoomed-in view on the grid near the Bahamas, where local refinements are applied to resolve steep slopes; (d) vertical grid along a transect from the Chesapeake Bay mouth to the continental slope. The whole grid is too dense to present; the mesh in the open ocean is largely uniform, similar to the configuration in the deeper part of (c).

et al. (1995) and Budgell et al. (2007). The rectangular domain is 10^7 m from the western boundary to the east boundary and 6.3×10^6 m from the south boundary to the north boundary (Fig. 9a). The steady flow field has the following stream function (see streamlines in Fig. 9a):

$$\Psi = \frac{1}{\rho} \gamma \left(\frac{b}{\pi} \right)^2 \sin \left(\frac{\pi y}{b} \right) (p e^{Ax} + q e^{Bx} - 1), \quad (17)$$

where x and y are cartesian coordinates pointing eastward and northward respectively, with the origin at the south-west corner of the domain; $b = 6.3 \times 10^6$ m is the meridional dimension; $\rho = 10^3$ kg m $^{-3}$ is the fluid density. The quantity γ is evaluated as:

$$\gamma = \frac{F\pi}{rb}, \quad (18)$$

where $F = 0.1$ N m $^{-2}$ is the surface wind stress; $r = 10^{-6}$ s $^{-1}$ is the frictional coefficient. Other coefficients are expressed as:

$$A = -\frac{\alpha}{2} + \left[\frac{\alpha^2}{4} + \left(\frac{\pi}{b} \right)^2 \right]^{1/2}, \quad (19)$$

$$B = -\frac{\alpha}{2} - \left[\frac{\alpha^2}{4} + \left(\frac{\pi}{b} \right)^2 \right]^{1/2}, \quad (20)$$

$$p = \frac{1 - e^{B\lambda}}{e^{A\lambda} - e^{B\lambda}}, \quad (21)$$

$$q = 1 - p, \quad (22)$$

with

$$\alpha = \frac{1}{r} \frac{\partial f}{\partial y}, \quad (23)$$

where $f = y \times 10^{-11}$ m $^{-1}$ s $^{-1}$ specifies the f -plane location; $\lambda = 10^7$ m is the zonal width of the domain. The velocity is found from the volume transport stream function as:

$$u = D^{-1} \frac{\partial \Psi}{\partial y}, \quad (24)$$

$$v = -D^{-1} \frac{\partial \Psi}{\partial x}, \quad (25)$$

where $D = 200$ m is the water depth. The initial concentration (T_0) is a Gaussian hill specified by Eq. (16), with $x_0 = \lambda/3$, $y_0 = b/3$ and $\sigma = 800/\sqrt{2}$ km. The Gaussian hill is advected by the steady flow field for a total duration of 1.5×10^8 s (about 5 years) with a model time step of 2×10^4 s.

We used a nearly uniform triangular grid (Fig. 9b) with a resolution of 105 km, close to the uniform grids in Hecht et al. (1995) and Budgell

et al. (2007), but these grids are not identical because of different gridding techniques. We chose SMS as the grid generator so that the final grid resembles that in a realistic eddying-ocean application (cf. Section 4.2 and the deep region in Fig. 10c). The results were compared with a reference solution (Fig. 9d) obtained from a sixth-order Runge–Kutta backtracking based on Eqs. (24) and (25). The following statistics were used for model assessment:

$$\text{MIN} = \min\{T\} - \min\{T_R\}, \quad (26)$$

$$\text{MAX} = \max\{T\} - \max\{T_R\}, \quad (27)$$

$$l_2 - \text{norm} = \left\{ \frac{\overline{(T - T_R)^2}}{\overline{T_R^2}} \right\}^{\frac{1}{2}}, \quad (28)$$

$$\text{Variance} = \overline{(T - \bar{T})^2} / (\overline{T_R - \bar{T}_R})^2 - 1, \quad (29)$$

where T is the simulated concentration, T_R is the reference solution, and the overbar denotes area-weighted average.

The final concentration field on the 105-km resolution grid at the end of the 5-year simulation is shown in Fig. 9e., which is similar to that of the FCT (flux-corrected transport) schemes in Hecht et al. (2000) and Budgell et al. (2007). With this coarse resolution, the shape and peak were only modestly preserved, with $\text{MIN} = -0.046$, $\text{MAX} = -0.633$, $l_2 - \text{norm} = 0.728$ and $\text{Variance} = -0.681$, which are slightly worse than the FCT results. In Budgell et al. (2007), improved results were obtained with a variable resolution UG with grid size ranging from 7.4 km to 219 km. Since this UG is not available to us, we used another finer quasi-uniform grid with 40-km resolution. Compared to the coarse grid, the simulated concentration on the finer grid (Fig. 9f) is much closer to the reference solution and also to other models with the variable resolution UG (Budgell et al., 2007).

4. Application to the Gulf stream

4.1. Background

The new transport solver was next put into test in a realistic application, with a regional domain covering the north-west Atlantic off the US east coast, the Gulf of Mexico, and the Caribbean Sea (Fig. 10a). Local mesh refinements were applied in the Chesapeake Bay and the adjacent mid-Atlantic Bight (MAB), mainly to test the new solver's efficiency under large grid-size transitions, as well as robustness under both eddying and non-eddying regimes. Large-scale baroclinic ocean processes are the focus here. On the MAB, the mean equator-ward flowing shelf current and shelf break jet are strong signals on the shelf, while the poleward flowing Gulf Stream dominates the upper ocean flow field seaward of the shelf break (e.g., Chen and He, 2015). The Gulf Stream path veers towards the open ocean near Cape Hatteras where the current begins to shift from a topographically steering western boundary current to a vigorously meandering free jet. Recent observations suggest that the increasing variability of this separation point may be a plausible cause for the warming of the MAB and local relative sea-level rise (Andres, 2016; Ezer et al., 2013). This baroclinic instability creates complex eddies and counter-currents (Chen et al., 2014a). The variability in Gulf Stream location and its associated shelf intrusion, meandering, and eddy shedding are active research topics in the ocean modeling community (e.g., Chen et al., 2014b). So far, most of the modeling efforts are based on SG models (e.g., Chen and He, 2015; Zeng and He, 2016), where *bathymetry smoothing* at large slopes and *grid nesting* in coastal regions are often required. Successfully applying a multi-resolution UG model to this system has two major benefits. First, it allows steep bathymetry (e.g., submarine canyons) to be faithfully represented with high resolution. Recently developed techniques in SCHISM (Zhang et al., 2015, 2016) ensure that the accuracy and efficiency of a baroclinic simulation are not compromised for flows over steep bathymetry. Second, it facilitates the simulation of estuary–ocean exchange when high resolution in

coastal areas is needed. For an SG model, two or more layers of grid-nesting are typically required to transition km-scale grid size in the ocean to meter-scale grid size in coastal regions (Mason et al., 2010; Dauhajre and McWilliams, 2019), whereas a recent SCHISM baroclinic application resolves small-scale structures at 1-m resolution within an estuary-to-shelf domain with a time step of 120 s (Liu et al., 2018).

4.2. Model setup

The spatial domain (Fig. 10a) was discretized by an unstructured grid with 430 K nodes and 840 K elements in the horizontal dimension (see illustrations in Fig. 10bc). A resolution of 6–7 km was applied in the open ocean, which smoothly transitioned to about 2 km near the coastline and down to 100 m inside the Chesapeake Bay. The vertical grid adopted the terrain following LSC² coordinate (Zhang et al., 2015) with depth-dependent layer numbers (27.0 layers on average and 44 layers in the deepest ocean; Fig. 10d). Atmospheric forcing from North American Regional Reanalysis (NARR²) was applied at the surface, including air temperature, surface pressure, humidity, wind speed and direction, short-wave and long-wave radiation. To filter out the spurious inertial modes that often arise in UG models (Ringler et al., 2010; Danilov, 2012), a bi-harmonic viscosity was used in the horizontal momentum advection scheme (Zhang et al., 2016). In addition, a Shapiro filter (Shapiro, 1970) is locally applied at steep slopes where the spurious modes are most severe, for example in the region shown in Fig. 10c. The Shapiro filter strength (γ ; non-dimensional) is specified based on the bathymetric slopes (α ; non-dimensional) as $\gamma = 0.5 \tanh(\frac{\alpha}{\alpha_0})$, where α_0 is a reference slope taken to be 0.5 in this case. This leads to a maximum filter strength of 0.5 for bathymetric slopes exceeding 0.5. Horizontal diffusivity was not explicitly applied; and the vertical viscosity/diffusivity is calculated by the generic length-scale model ($k - kl$; Umlauf and Burchard, 2003). Initialized from the HYCOM reanalysis product on April 1, 2012, the model ran for 110 days with a time step of 150 s. The simulation speed was 190 times faster than real time, using 540 Intel Xeon cores (Broadwell E5-2695 v4 @ 2.1 GHz). Since the initial condition was derived from HYCOM, the model was considered properly spun up after 2 weeks (similar to Zeng and He, 2016). It is worth noting that the model setup differs from standard SG models mainly in four aspects:

- (1) large element size transition from estuaries (100 m) to the open ocean (7 km) in a single grid;
- (2) original non-smoothed bathymetry captured with local refinements at steep slopes (Fig. 10c);
- (3) depth-varying but terrain-following vertical layers (Fig. 10d);
- (4) no data assimilation.

4.3. Model assessment

The regional SCHISM model with the setup described in Section 4.2 using the new transport solver is referred to as the “base model” in this study. The results from the base model were validated against the observed sea surface height (SSH) from AVISO global sea surface height product³ and sea surface temperature (SST) from NASA's GHRSSST Level 4 G1SST global foundation sea surface temperature analysis.⁴ Since a comprehensive model assessment for the Gulf Stream is beyond the scope of this paper, we only present the comparisons on the most important variables, including: (1) the time series of the error statistics for SSH and SST throughout the domain; (2) vertical temperature

² Url: <https://www.esrl.noaa.gov/psd/data/gridded/data.narr.html>, last accessed in April 2019.

³ Url: <https://www.aviso.altimetry.fr/en/data/products/sea-surface-height-products/global.html>, last accessed in June 2019.

⁴ Url: https://podaac.jpl.nasa.gov/dataset/JPL_OUROCEAN-L4UHFnd-GLOB-G1SST, last accessed in June 2019.

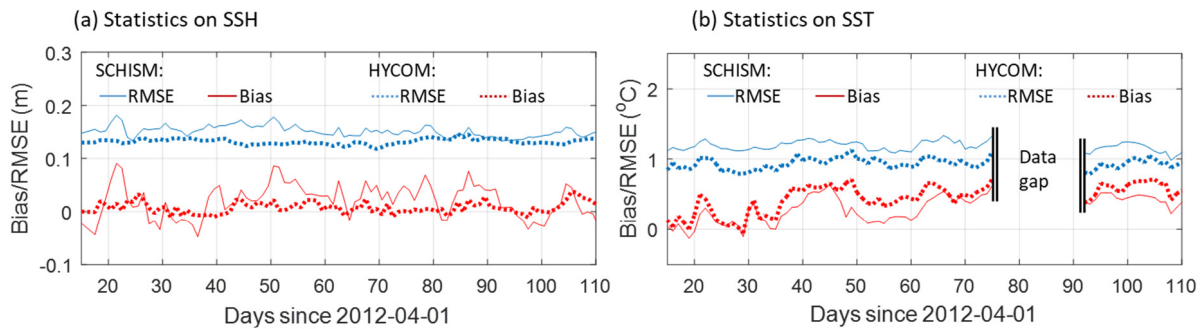


Fig. 11. Error statistics including bias and root mean square error (RMSE) for the base model (SCHISM) and the global model HYCOM on: (a) SSH; (b) SST (with a 15-day gap in the observation data).

profiles at Argo⁵ casts near the Gulf Stream; and (3) SST snapshots near the end of the simulation period when Gulf Stream develops strong meanders.

The time series of model error (root mean square error and bias) calculated over the entire model domain indicate the base model is slightly worse in SSH and SST skills than HYCOM (Fig. 11). This is expected since HYCOM applies data assimilation, which may also be the reason that HYCOM's error statistics on SSH show smaller temporal variations than SCHISM's. In general, both models over predict SST during this spring–summer period, which is likely due to the uncertainties in the atmospheric forcing. Overall, the base model is deemed capable of realistically capturing the general trend in SSH and SST; its similar skill to the data-assimilated HYCOM lends further confidence.

As an important variable delineating the Gulf Stream signature, 3-D temperature was further validated against Argo data. This dataset consists of randomly located vertical profiles from surface to 2000-m depth that spread out the model domain. Fig. 12 shows the comparisons on selected floats near the Gulf Stream course in July 2012, a period with strong meanders that are challenging for the model. The simulated 3-D temperature matches most of the observed profiles well, with an overall RMSE (root mean square error) of 1.47 °C and an overall CC (correlation coefficient) of 0.99. The skill is very close to the data-assimilated HYCOM results, which have an overall RMSE of 1.48 °C and an overall CC of 0.98. Larger errors are noticeable near the east ocean boundary (the 13th and 14th profiles in Fig. 12). This may be due to the base model trying to reconcile its interior solution with the boundary condition forced by HYCOM, which itself has uncertainty.

Sensitivity runs of the base model were then conducted to assess the relative performance between the new 3rd-order WENO scheme and the old 2nd-order TVD scheme. In particular, the performances in the following two aspects are critical for a successful baroclinic simulation in the eddying regime.

The first aspect is the intensity of the simulated relative vorticity, which is a good indicator of a model's capability in resolving baroclinic instability. The simulated vorticity in the Atlantic Ocean at the end of the 110-day simulation are presented in Fig. 13. The patterns are generally consistent between the two schemes, where the Gulf Stream core is identified by the large vorticity magnitudes. Compared to the relatively smooth features simulated by the lower-order scheme, the new scheme generates more energetic and sharply defined flow and eddying patterns, corresponding to a 23% increase in eddy kinetic energy at the end of the simulation.

The second aspect is on 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; Chen and He, 2015). As the temperature rises in summer (about 90 days into the simulation period), the Gulf Stream starts to develop strong meanders after separating from the shelf near

Cape Hatteras. At least one eddy formation event is visible during this period, as part of a strong meander folds on itself (highlighted by the black arrow in Fig. 14a). These features were not clearly captured by the old scheme as shown in Fig. 14c & g, in which the signature of the Gulf Stream is too diffuse; in contrast, the new scheme qualitatively captured this event (Fig. 14d & h) and resolved the eddies and filaments in greater detail. In fact, the results from the new scheme seem not diffusive enough and tend to exaggerate the meanders and eddy detachments, as compared with the observation (Fig. 14h) and the data-assimilated HYCOM (Fig. 14f). The main cause is that the SCHISM runs have a positive bias in SST in the region shown in Fig. 14g & h, as well as the whole domain (Fig. 14c & d). As a result, the simulated SST from the SCHISM runs exhibits larger errors than HYCOM within this region (see statistics for Fig. 14f–h). The surface over-heating issue is expected to be corrected by further calibrations on the parameters of air–sea heat exchange, which is left for future studies focusing on Gulf Stream dynamics.

In this application, the numerical dispersion (i.e. spurious concentration patterns) is small enough, so no additional filtering or artificial diffusion is applied for the tracer transport in the eddying regime. In the non-eddy regime such as shallow waters, a practical solution for minor dispersion issues is to transition to the 1st-order upwind scheme when the local water depth is below a given threshold (e.g. 5 m). For the commonly used advection schemes in ocean models, there are other approaches to eliminate oscillations (Budgell et al., 2007), and we have experimented with some filters such as ELAD (Shchepetkin and McWilliams, 1998). We choose not to use them in the new transport scheme for now, because they would degrade the order of accuracy in the eddying regime.

5. Conclusions

In this paper, a 3rd-order transport scheme based on WENO has been designed for improving the utility and skill of SCHISM in simulating baroclinic circulation in open ocean eddying regime. The specific designs focus on striking a delicate balance among accuracy, monotonicity, efficiency, and robustness. We show that baroclinic eddies and filaments are better resolved with this new scheme. In the idealized benchmark tests and the realistic Gulf Stream simulation, we have demonstrated that the new 3rd-order scheme is capable of better controlling numerical dissipation, maintaining sharp frontal instabilities, and resolving major baroclinic circulation and eddying features associated with the Gulf Stream. In all experiments, the 3rd-order scheme outperformed the 2nd-order TVD scheme, with a moderate increase of 20%–30% in computational time. Explicit diffusion or diffusive filters, which control numerical dispersion but essentially degrade accuracy, were not applied in these experiments. Nevertheless, minor over/under-shoots can happen locally in a large gradient zone (e.g., in shallow waters), since the scheme is “essentially non-oscillatory”, but these are minor enough to be tolerated by the model, and the issue can also be mitigated by transitioning to lower-order schemes in shallow waters.

⁵ Url: <http://www.argo.ucsd.edu/>, last accessed in January 2019.

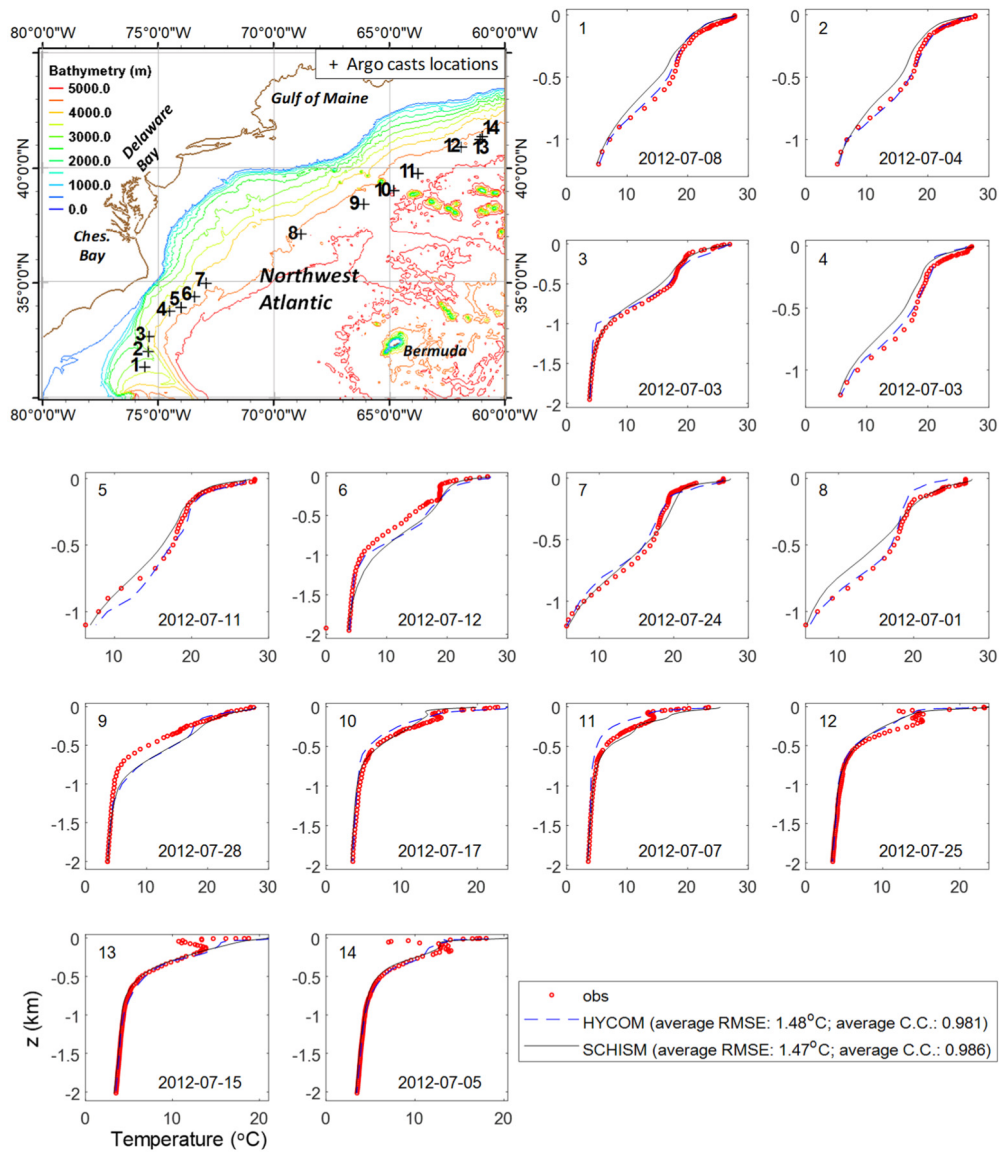


Fig. 12. Model-data comparison of 3-D temperature in July 2012. The locations of Argo floats are shown in the top-left panel. The vertical profiles are arranged geographically (from west to east).

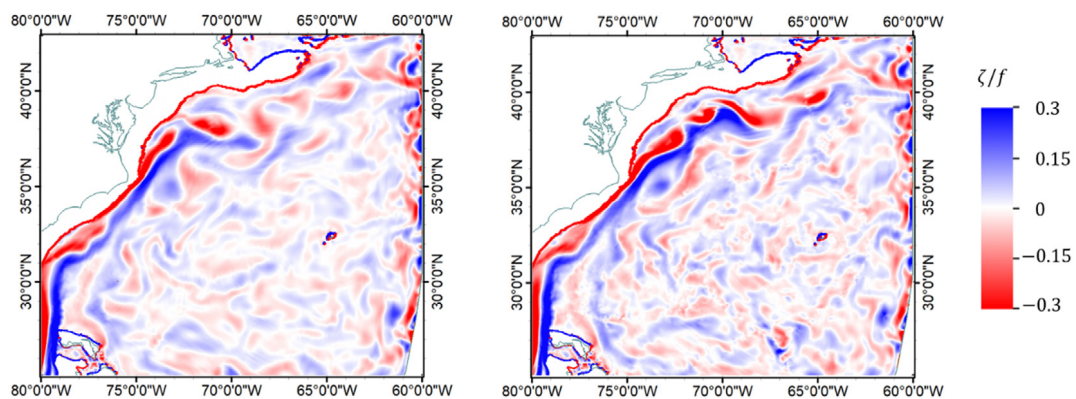


Fig. 13. Simulated relative vorticity (scaled by Coriolis parameter) at $z = -100$ m (cut off at shelf break) at the end of the simulation: (a) 2nd-order TVD; (b) 3rd order WENO.

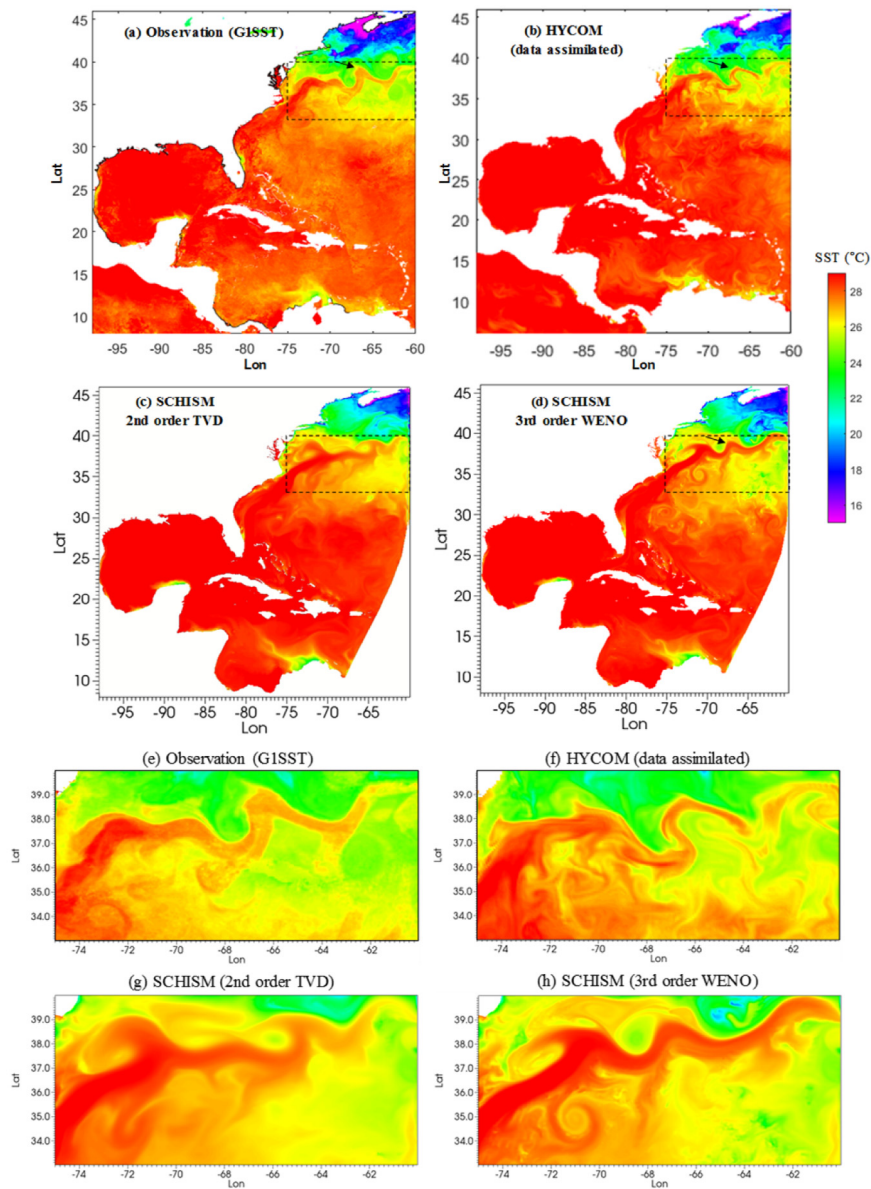


Fig. 14. SST patterns near the end of the simulation period (Day 106; July 16, 2012), representative of the condition with strong meanders in the Gulf Stream (with the black arrow pointing to a part of the meander that starts to fold on itself): (a) observation; (b) HYCOM with data assimilation; (c) SCHISM with 2nd-order TVD for transport; (d) SCHISM with 3rd-order WENO for transport; (e) zoomed-in views of (a); (f) zoomed-in views of (b), MAE = 0.7 °C; (g) zoomed-in views of (c), MAE = 1.4 °C; (h) zoomed-in views of (d), MAE = 1.1 °C. The statistics are calculated over the zoomed-in region.

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