Exploring Salinity Issues in the Texas Coast using SELFE: Semi-Implicit Finite-Element/Volume Eulerian-Lagrangian algorithm

Report
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Texas Water Development Board

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1 Executive Summary

Despite significant advances in coastal ocean models, including improvements in model physics, numerical algorithms, grid resolution, and data inputs, we still experience difficulty in accurately modeling freshwater/saltwater interfaces. This is particularly true in Texas bays and estuaries where freshwater inflows are sporadic and salinity is influenced by tides, evaporation, wind and other factors [2]. This report contains the work done to improve the TWDB's capabilities to model salinity transport in transition regions where freshwater and saltwater interact. New transport methods were investigated using SELFE (Semi Eulerian-Lagrangian Finite Element method) software and a new version of SELFE, which include Finite Volume formulations. Improvements in the modeled salinity levels compared with observed data were made, the relevant results and processes of which are described below. At the end of this report are included user instructions for conducting salinity studies using SELFE and on post-processing results using python based scripts.

2 Introduction

2.1 Background information

TWDB personnel conducted extensive research on mixing in the lower Brazos River and reported the following [3]:
"The Brazos River has a low-volume, mid-depth riverine estuary where freshwater inflow from the river and salt waters from the Gulf of Mexico mix creating a zone where salinity varies from marine salinity at the river mouth to freshwater at the upstream boundary of this zone. The Lower Brazos River upstream of the estuary is a freshwater source supporting industrial, municipal and irrigation uses in adjacent counties. This reach of the river supplies drinking water to the surrounding cities of Angleton, Brazoria, Clute, Freeport, Lake Jackson, Oyster Creek and Richwood. Dow Chemical and other nearby industrial facilities also rely on the freshwater resource of the Brazos River for their operation. The intake pipes that divert from the Lower Brazos River for these water rights are at the Brazoria Reservoir located at river mile 24 and William Harris Reservoir located at river mile 44. In the period from 1940 – 1960, the Lower Brazos River underwent several additional changes to its physical and hydrologic conditions. The construction of the Gulf Intercoastal Waterway was completed resulting in the connection of the Brazos River to the Freeport Channel to the north and San Bernard River to the south. The construction of William Harris and Brazoria reservoirs, both of which are off-channel storage reservoirs, was completed during this period. Dow Chemical Company Magnesium Plant construction adjacent to the river near the mouth also was completed during this period – this plant discharges saltwater to the river after cooling use. The potential impact of these changes to the salinity of the system is of interest because of biological activity and water supply. "

2.2 Research Description

The goal of this project was to investigate improvements to the transport algorithms within SELFE used for salinity and temperature transport, and investigate new high-resolution transport algorithms, which may help to eliminate the common smearing of freshwater/saltwater interfaces [2]. Before this project began, we were only aware of Eulerian-Lagrangian transport methods in SELFE. By the time the project started, some new transport algorithms, including second order TVD methods, had been added to SELFE by the lead developer Joseph Zhang. Testing these new methods became the focus of the project. The model was applied to the Brazos River region, using parameters specified by TWDB. For these test cases, in addition to testing various transport methods, we also tested mesh and time step refinement.

In year 2 of the project, we obtained a "beta" version of SELFE that was recently released. The majority of effort in year 2 was spent on compilation, grid adjustments and testing the new version of SELFE. This report, which includes the summary of the work conducted on this project, results and user instructions, is also part of the tasks completed in year 2.

3 SELFE

The Semi-implicit Eulerian-Lagrangian Finite Element (SELFE) model is an open-source community-supported code. It is based on unstructured triangular grids, and designed for the effective simulation of 3D baroclinic circulation. SELFE uses a semi-implicit finite-element/volume Eulerian-Lagrangian algorithm to solve the Navier-Stokes equations (in either hydrostatic or non-hydrostatic form). The numerical algorithm is high-order, robust, stable and computationally efficient (at least when executed on serial machines) due to its ability to take fairly large times steps. It also naturally incorporates wetting and drying of tidal flats [1].

3.1 Model Grid

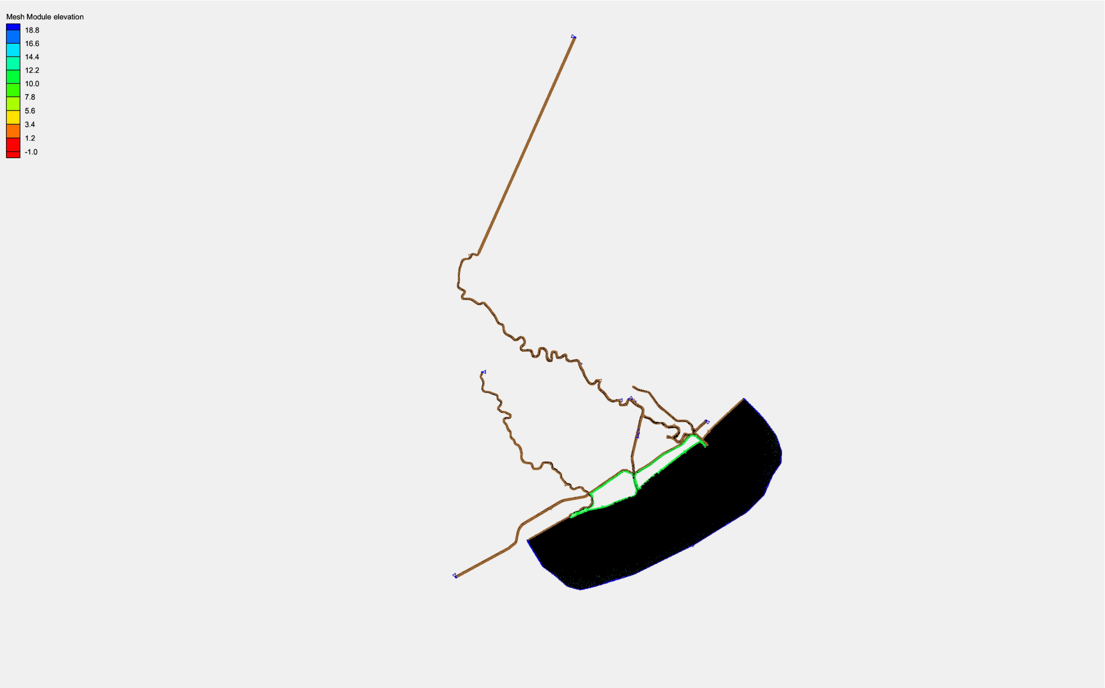


Figure 1. Brazos River Domain

As shown in the Figure 1 above the model domain incorporates the following systems: 35 river miles of the Brazos River and an additional 19 miles of "false" delta (a simplified representation of the unresolved portion of the river upstream of the SH 35 Bridge that was added to allow for accurate propagation of the tidal prism on the Brazos River), 20 river miles of the San Bernard River, parts of the Gulf Intracoastal Waterway (GIWW) adjacent to the Brazos and San Bernard Rivers, and adjacent Gulf of Mexico shelf [3].

An unstructured grid was constructed on this domain using the Surface Water Modeling System (SMS). The Gulf of Mexico portion of the model grid extended 6.5 miles offshore from the mouth of the Brazos River and 20 miles along the shoreline extending from 3.8 miles south of the old San Bernard River mouth to 4.5 miles north of Freeport Channel Entrance. The offshore distance of the open boundary was established at a location where little salinity variation was assumed to exist thus enabling a constant ocean salinity boundary condition specification for the simulation periods.

3.2 Model Configuration and Validation Overview

Various parameters will be given in the test case section of the report, specific to the cases described. Salinity data recorded from various monitoring sites were provided to the model for horizontally varying initial conditions. Vertically uniform salinity initial conditions were specified because SELFE allows for variation of initial conditions only in one plane. Velocity and water level were "cold started," where initial velocity values in the domain were set to zero, and the initial water level was set to mean sea level (MSL) uniformly throughout the model domain. Model stability and consistency were examined at various time step values as shown in the test cases section, and a value of 15 sigma layers was adopted for validation and scenario simulations [3,4]. **Figure 3** shows sites of the salinity recording stations and **Table 2** gives additional information.

Table 1. **Sigma levels (left) and Z-coordinates (right). Origin of the vertical axis is at MSL; h_c, theta_b, theta_f are constants used in Song and Haidvogel's (1994) S-coordinate system. h_c controls surface/bottom boundary layer thickness that requires fine resolution; theta_f-->0 leads to traditional sigma-coordinates, while theta_f >> 1 skews resolution towards surface and/or bottom; theta_b=1 leads to both bottom and surface being resolved, while theta_b=0 resolves only surface [4].**

Figure 2 **depicts this geometry.**

6. 0. 3. !h_c, theta_b, theta_f	
1	-1.
2	-0.933333
3	-0.866667
4	-0.800000
5	-0.733333
6	-0.666667
7	-0.600000
8	-0.533333
9	-0.466667
10	-0.400000
11	-0.333333
12	-0.266667
13	-0.200000
14	-0.133333
15	-0.066667
16	0.

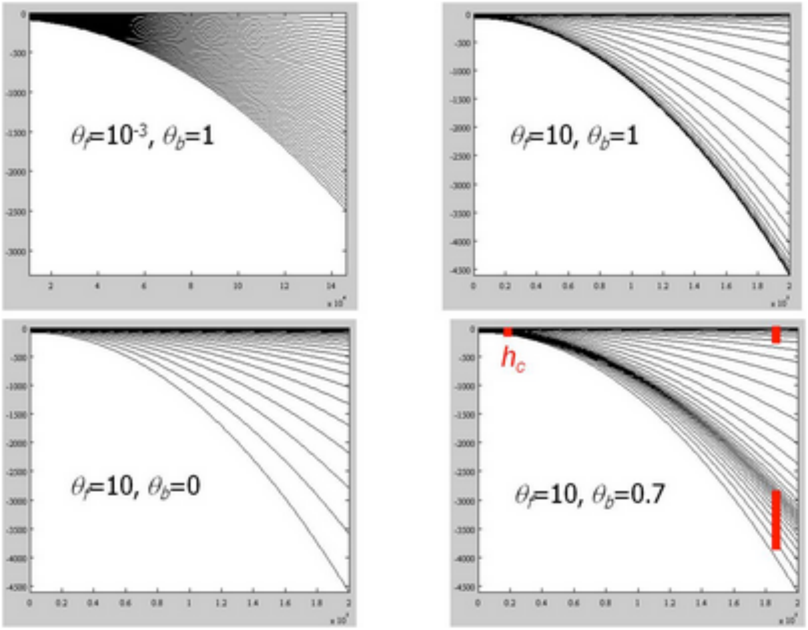
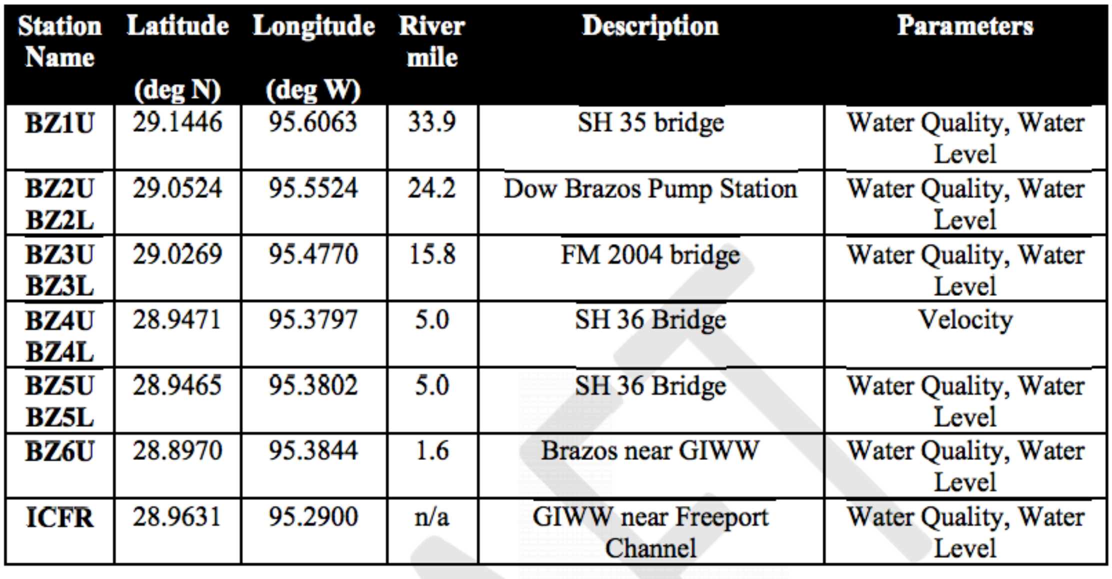


Figure 2. **h_c, theta_b and theta_f [4]**

Table 2. **Salinity monitoring site info [3].**



Station Name	Latitude (deg N)	Longitude (deg W)	River mile	Description	Parameters
BZ1U	29.1446	95.6063	33.9	SH 35 bridge	Water Quality, Water Level
BZ2U **BZ2L**	29.0524	95.5524	24.2	Dow Brazos Pump Station	Water Quality, Water Level
BZ3U **BZ3L**	29.0269	95.4770	15.8	FM 2004 bridge	Water Quality, Water Level
BZ4U **BZ4L**	28.9471	95.3797	5.0	SH 36 Bridge	Velocity
BZ5U **BZ5L**	28.9465	95.3802	5.0	SH 36 Bridge	Water Quality, Water Level
BZ6U	28.8970	95.3844	1.6	Brazos near GIWW	Water Quality, Water Level
ICFR	28.9631	95.2900	n/a	GIWW near Freeport Channel	Water Quality, Water Level

Figure 3. **Salinity monitoring sites (Google Earth view).**

3.3 Model Boundary conditions

Table 3. Model boundary information.

Name	# of nodes in boundary	elevation boundary flag	flux boundary flag	temperature boundary flag	Salinity boundary flag
Brazos River	7	0	1	0	2
San Bernard River	5	0	1	0	2
Giww-west	5	2	0	0	2
Ocean	449	1	0	0	2
Giww-east	7	2	0	0	2
Return @7536 ups giww	2	0	1	0	2
return@33332 downs dow	2	0	1	0	2
return @6483-001A dow1	2	0	1	0	2
return @6483-002A + 6483-003A dow2 and 3	2	0	1	0	2
return @8788 ups of dow	2	0	1	0	2
return @25798 ups of dow2	2	0	1	0	2

The number codes in the above table correspond to the following [4]:

0- nothing specified

1- time history read from *.th file where * could be elevation, flux, temperature or salinity.

2- Constant value for the boundary

3- Boundary is forced by tides

4- time history of value on this boundary

Figure 4 shows Brazos River boundaries of the grid as observed from Google Earth.

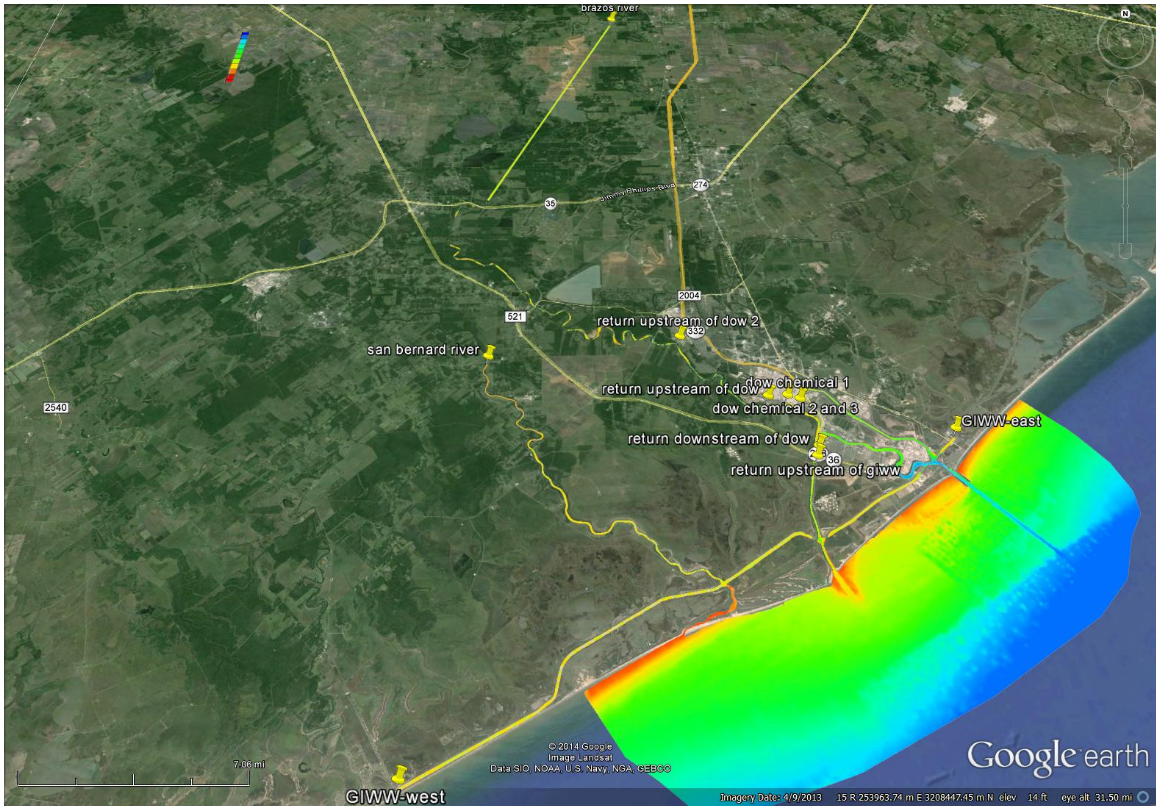


Figure 4. **Brazos river boundaries (Google earth view)**

3.3.1 Tides

No tidal harmonics were specified, but a time-varying water level time-series at 6 minute frequency was specified. This should capture tidal and residual variation.

3.3.2 Meteorology

In some test cases, a periodic wind forcing was introduced. The time history of the wind-forcing file has the following format:

Table 4. **Wind speed input format.**

X component	Y component
-.44	1.54
-.44	1.54

3.3.3 Salinity

Lack of sufficient salinity data needed to specify boundary conditions presented a challenge in this modeling effort. In the case of the Gulf of Mexico boundary, this was overcome by extending the model domain six miles offshore to an interface where the boundary condition could be forced with constant salinity [3]. For other boundaries, either a constant value or time history values were specified, which are noted in the cases below.

3.4 Physical formulation

These formulations were taken from the paper published on SELFE, and Joseph Zhang's notes and presentations on SELFE [5,6].

3.4.1 Governing equations: Reynolds-averaged Navier-Stokes:

Continuity: $$\nabla \cdot \mathbf{u} + \frac{\partial w}{\partial z} = 0,\ (\mathbf{u} = (u, v))$$

$$\frac{\partial \eta}{\partial t} + \nabla \cdot \int_{-h}^{\eta} \mathbf{u} dz = 0$$

$$-\frac{\partial \rho}{\partial t} = \frac{\partial (\rho u)}{\partial x} + \frac{\partial (\rho v)}{\partial y} + \frac{\partial (\rho w)}{\partial z}$$

$$= \nabla_3 \cdot (\rho \mathbf{u})$$

(Eulerian Form)

$$\boxed{\frac{\partial \rho}{\partial t} + \nabla_3 \cdot (\rho \mathbf{u}) = \frac{D\rho}{Dt} + \rho \nabla_3 \cdot \mathbf{u} = 0}$$

(Lagrangian Form)

3.4.2 Momentum:

$$\frac{D\mathbf{u}}{Dt} = \mathbf{f} - g\nabla\eta + \frac{\partial}{\partial z}\left(\nu \frac{\partial \mathbf{u}}{\partial z}\right); \quad \mathbf{f} = -f\mathbf{k} \times \mathbf{u} + \alpha g \nabla \hat{\psi} - \frac{1}{\rho_0}\nabla p_A - \frac{g}{\rho_0}\int_z^{\eta} \nabla \rho d\zeta + \nabla \mathbf{g}(\mu \nabla \mathbf{u})$$

$$\frac{D\mathbf{u}}{Dt} = -\frac{1}{\rho}\nabla P + \nabla_3 \cdot (\nu \nabla_3 \mathbf{u}) - f\mathbf{k} \times \mathbf{u}$$

$$\frac{Dw}{Dt} = -\frac{1}{\rho}\frac{\partial P}{\partial z} - g + \nabla \cdot (\nu \nabla w)$$

(Lagrangian form)

Equation of state: $\rho = \rho(p, S, T)$

3.4.3 Transport of salt and temperature:

$$\frac{Dc}{Dt} = \frac{\partial}{\partial z}\left(\kappa \frac{\partial c}{\partial z}\right) + \dot{Q} + \nabla\cdot(\kappa_h \nabla c), \quad c = (S,T)$$

3.4.4 Transport boundary conditions:

$$\kappa \frac{\partial c}{\partial z} = \hat{c}, \quad z = \eta$$

$$\kappa \frac{\partial c}{\partial n} = 0, \quad z = -h$$

3.4.5 Momentum vertical boundary conditions:

$$\nu \frac{\partial \mathbf{u}}{\partial z} = \boldsymbol{\tau}_w \ \text{ at } \ z{=}\eta \quad \text{(surface)}$$

$$\nu \frac{\partial \mathbf{u}}{\partial z} = C_D \,|\,\mathbf{u}_b\,|\,\mathbf{u}_b, \ \text{ at } \ z = -h \quad \text{(bottom)}$$

3.4.6 Reynolds stress:

$$\boxed{\nu \frac{\partial \mathbf{u}}{\partial z} = \frac{\kappa_0}{\ln(\delta_b / z_0)} C_D^{1/2} \,|\,\mathbf{u}_b\,|\,\mathbf{u}_b, \quad (z_0 - h \le z \le \delta_b - h)}$$

3.4.7 Drag Coefficient:

$$C_D = \left(\frac{1}{\kappa_0} \ln \frac{\delta_b}{z_0}\right)^{-2}$$

3.4.8 Turbulence Models:

There were a few turbulence models tested within SELFE. A typical formulation is described below.

Mellor-Yamada-Galperin (1988): This model assumes that the turbulence mixing is related to the growth and dissipation of turbulence kinetic energy (k) and Monin-Obukhov mixing length (l); k and l are derived from the 2nd moment turbulence theory.

$$\frac{Dk}{Dt} = \frac{\partial}{\partial z}\left(\nu_k \frac{\partial k}{\partial z}\right) + \nu M^2 + \kappa N^2 - \varepsilon$$

$$\frac{D(kl)}{Dt} = \frac{\partial}{\partial z}\left(\nu_k \frac{\partial (kl)}{\partial z}\right) + \frac{lE_1}{2}\left(\nu M^2 + \kappa N^2\right) - \Psi \frac{\varepsilon l}{2}$$

Dissipation rate:

$$\varepsilon = \frac{(2k)^{3/2}}{B_1 l}$$

Shear and Buoyancy frequency:

$$M^2 = \left(\frac{\partial u}{\partial z}\right)^2 + \left(\frac{\partial v}{\partial z}\right)^2$$

$$N^2 = \frac{g}{\rho_0}\frac{\partial \rho}{\partial z}$$

Viscosity and diffusivities:

$$\nu = s_m (2k)^{1/2} l$$

$$\kappa = s_h (2k)^{1/2} l$$

3.5 Numerical formulation

SELFE uses a semi-implicit finite element framework. There are also options of using conformal vs. non-conformal shape functions. We tested both and listed in the results sections are the optimal options [6].

Continuity: $$\frac{\eta^{n+1} - \eta^n}{\Delta t} + \theta \nabla g \int_{-h}^{\eta} \mathbf{u}^{n+1} dz + (1-\theta) \nabla g \int_{-h}^{\eta} \mathbf{u}^n dz = 0$$

$$\boxed{\int_{\Omega} \left[\phi_i \eta^{n+1} + g\theta^2 \Delta t^2 \hat{H}^n \nabla \phi_i g \nabla \eta^{n+1}\right] d\Omega - g\theta^2 \Delta t^2 \int_{\Gamma_v} \phi_i \hat{H}^n \frac{\partial \eta^{n+1}}{\partial n} d\overline{\Gamma}_v + \theta \Delta t \int_{\Gamma_v} \phi_i \hat{U}_n^{n+1} d\Gamma_v = I^n}$$

Momentum: $$\frac{\mathbf{u}^{n+1} - \mathbf{u}_*}{\Delta t} = \mathbf{f}^n - g\theta \nabla \eta^{n+1} - g(1-\theta)\nabla \eta^n + \frac{\partial}{\partial z}\left(\nu^n \frac{\partial \mathbf{u}^{n+1}}{\partial z}\right)$$

Boundary conditions: $$\begin{cases} \nu^n \dfrac{\partial \mathbf{u}^{n+1}}{\partial z} = \boldsymbol{\tau}_w^{n+1}, \text{ at } z = \eta^n; \\ \nu^n \dfrac{\partial \mathbf{u}^{n+1}}{\partial z} = \chi^n \mathbf{u}_b^{n+1}, \text{ at } z = -h, \end{cases}$$

For transport methods, SELFE has the option of using Eulerian-Lagrangian, first order upwind or second order TVD methods. The Eulerian-Lagrangian and upwind methods have been used by TWDB in past studies. This method does not conserve mass and has been observed to be numerically diffusive. Upwind and TVD methods have been developed to help preserve steep solution gradients without sacrificing stability. The main focus of this project was testing the upwind and TVD methods. The current release version of SELFE allows for the use of upwind methods over the whole domain, and switches to a 2nd order TVD method in wetting and drying areas. The switch is determined by a minimum water depth parameter. This was the method used for most of the verification cases described below. The latest "beta" version of SELFE, which we also tested, allows for the use of the 2nd order TVD method over the whole domain.

The finite volume discretization of transport equation leads to the following upwind scheme:

$$V_i \frac{T_i^{m+1} - T_i^m}{\Delta t'} + \sum_{j \in \partial V}^{5} u_j S_j T_{j*} = V_i\, Q_{i,k}^m + A_i \Delta t' \left[\kappa_{i,k} \frac{T_{i,k+1}^{m+1} - T_{i,k}^{m+1}}{\Delta z_{i,k+1/2}} - \kappa_{i,k-1} \frac{T_{i,k}^{m+1} - T_{i,k-1}^{m+1}}{\Delta z_{i,k-1/2}} \right] +$$
$$\Delta t' \sum_{j=1}^{3} (\kappa_h)_j \frac{T_j^m - T_i^m}{\delta_{ij}} S_j, \quad (k = k_b + 1, \ldots, N_z)$$

In a similar manner, we also arrive at the TVD scheme for the transport equation:

$$T_i^{m+1} = T_i + \frac{\Delta t'}{V_i} \sum_{j \in S^-} |Q_j| \left(1 - \frac{\varphi_j}{2} \right) (T_j - T_i) + \frac{\Delta t'}{V_i} \delta \sum_{j \in S^-} |Q_j| \frac{\varphi_j}{2} (T_j - T_i) =$$
$$T_i \left[1 - \frac{\Delta t'}{V_i} \sum_{j \in S^-} |Q_j| \left(1 - \frac{\varphi_j}{2} + \delta \right) \right] + \frac{\Delta t'}{V_i} \sum_{j \in S^-} |Q_j| \left(1 - \frac{\varphi_j}{2} + \delta \right) T_j$$

3.6 Overview of the parallel code structure

We mainly describe here the parallel domain decomposition and nomenclature in the code [6].

3.6.1 Domain decomposition

1) The domain is first partitioned into non-overlapping sub-domains (in element sense)
- sub-domain may not be contiguous

2) Then each sub-domain is augmented with 1 layer of ghost elements where exchange of info occurs
- residents (elements, sides, nodes)
- ghosts
- aquire_hgrid(.false.) in partition_hgrid(): initial partition based on naïve ordering of elements
- ParMetis lib
    - MPI-based parallel library that implements a variety of algorithms for partitioning and repartitioning unstructured graphs
    - based on the multilevel partitioning and fill-reducing ordering algorithms that are implemented in the serial package METIS
    - Optimal partitioning is obtained by minimizing the edge cuts
    - Adjustable parameters for optimal performance
- aquire_hgrid(.true.): final partitioning

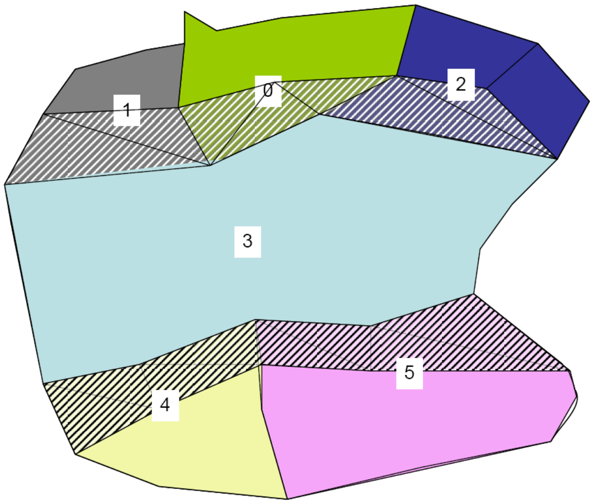


Figure 5- Domain decomposition [6].

3.62.2 Nomenclature

1) Each process (sub-domain) has its own set of variables
- global-to-local, local-to-global mappings
- resident vs augmented (i.e., resident + ghost)

2) Linked lists: iegl()%next%next%next…

- Each process has its own version of this list, with the local element number at the top (if inside aug. domain), and after that the rank numbers in ascending order
- ipgl and isgl(): interfacial nodes/sides will be resident in more than 1 domain
    - Consistency among processes (e.g., elevations): follow the smallest rank

3) Local vs ball info: need for exchange of info
- Computation usually done inside resident domain
- Communication done in ghost domain (expensive)

4) Communication
- MPI standard
- Bundle up before posting

5) Boundary info: all global info for simplicity

4 Test Cases

For the initial and second test case, the horizontal mesh used contained 76017 elements and 43273 nodes. For the refined grid case, the grid was modified using surface modeling solutions (SMS) through standard 2 levels of refinement upgrading the number of nodes to 153314, and number of elements to 291495.

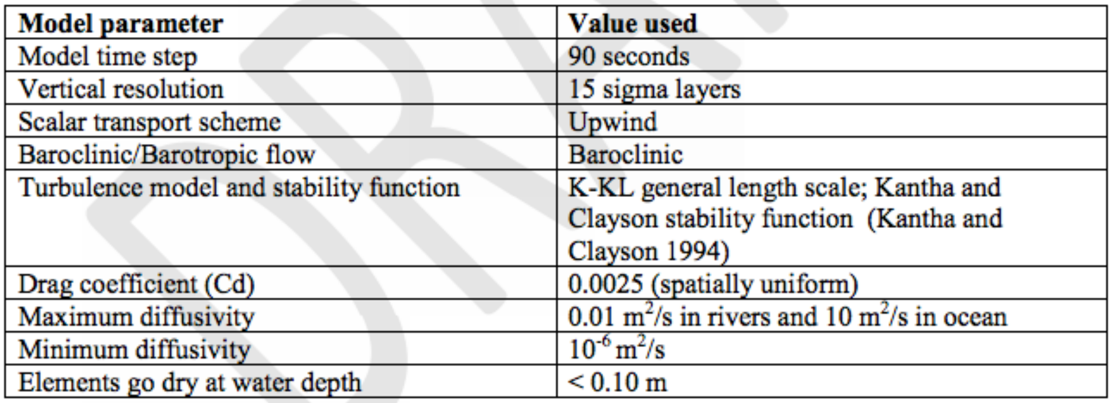
4.1 Initial studies

Before the project began, the following initial salinity studies were conducted by TWDB. In this study an upwind method was used for transport over the whole domain, the time step was 90 seconds and a K-KL general length scale turbulence model was used.

4.1.1 Model Configuration

Model parameters used in the study were as follows [3]:

Table 5. Model parameters for initial case



Model parameter	Value used
Model time step	90 seconds
Vertical resolution	15 sigma layers
Scalar transport scheme	Upwind
Baroclinic/Barotropic flow	Baroclinic
Turbulence model and stability function	K-KL general length scale; Kantha and Clayson stability function (Kantha and Clayson 1994)
Drag coefficient (Cd)	0.0025 (spatially uniform)
Maximum diffusivity	0.01 m^2/s in rivers and 10 m^2/s in ocean
Minimum diffusivity	10^{-6} m^2/s
Elements go dry at water depth	< 0.10 m

The next section shows time history plots from these studies.

4.1.2 Time History plots

As can be seen from Figures 6-10, the model typically over predicts or under predicts the salinities. It over predicts at BZ2U and BZ2L, BZ5U and BZ5L, and under predicts at BZ3U and BZ3L. These errors could be due to both numerical approximation errors and missing information. However, other factors such as inaccurate information about saltwater returns from surrounding reservoirs such as Harries and Brazoria reservoirs, and plants such as the Dow Chemical Co. plant could be part of the problem [3].

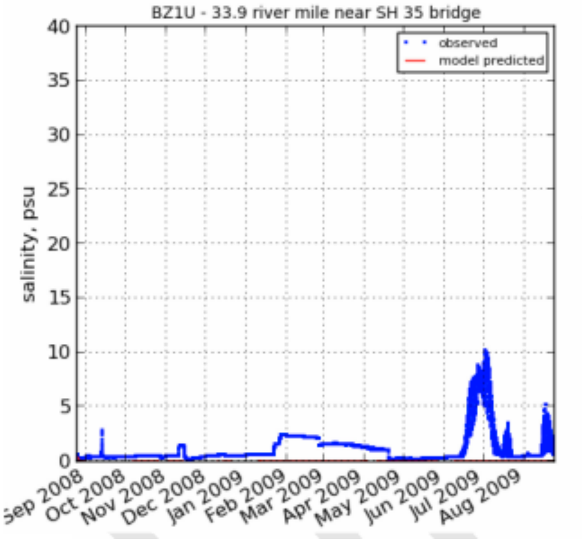


Figure 6. **Salinity at BZ1U [3]**

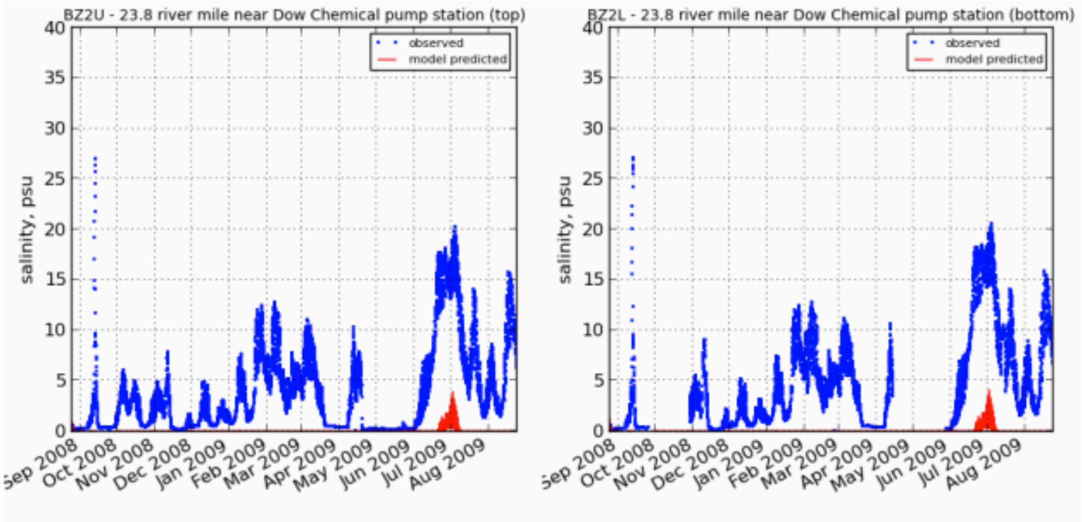


Figure 7. **Salinities at BZ2U and BZ2L [3]**

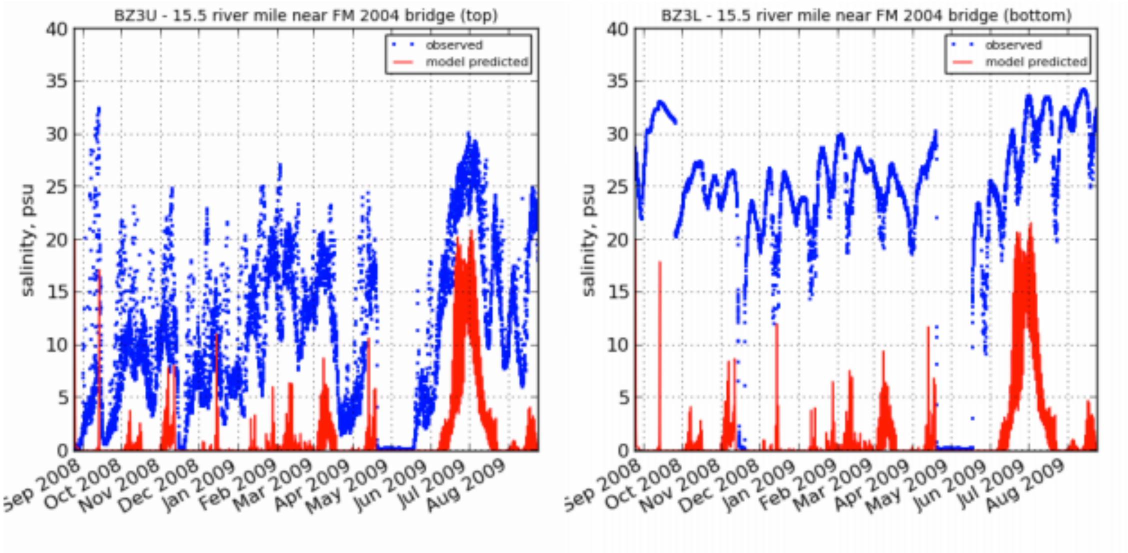


Figure 8. **Salinities at BZ3U and BZ3L [3]**

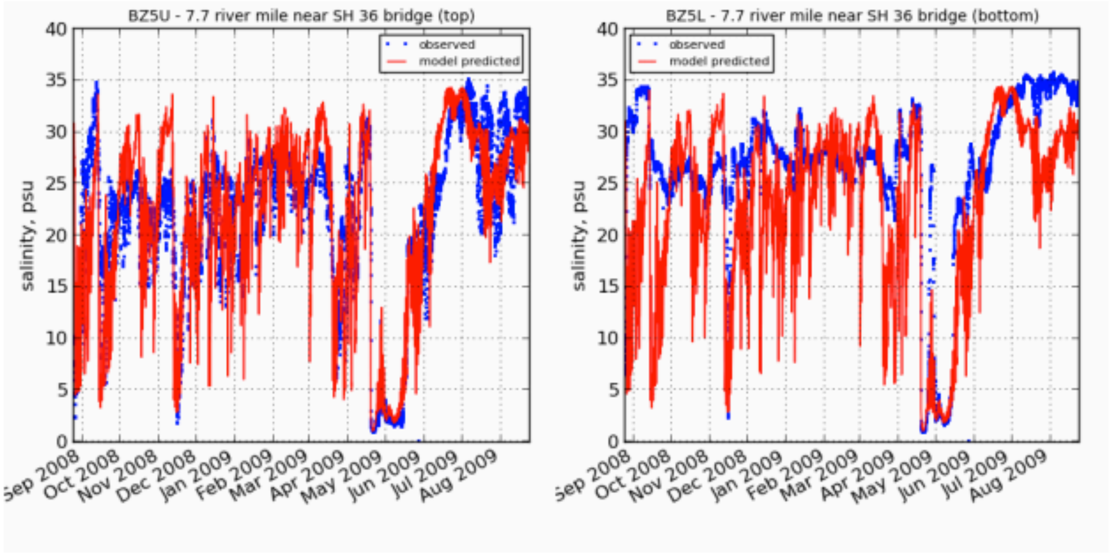


Figure 9. **Salinities in BZ5U and BZ5L [3]**

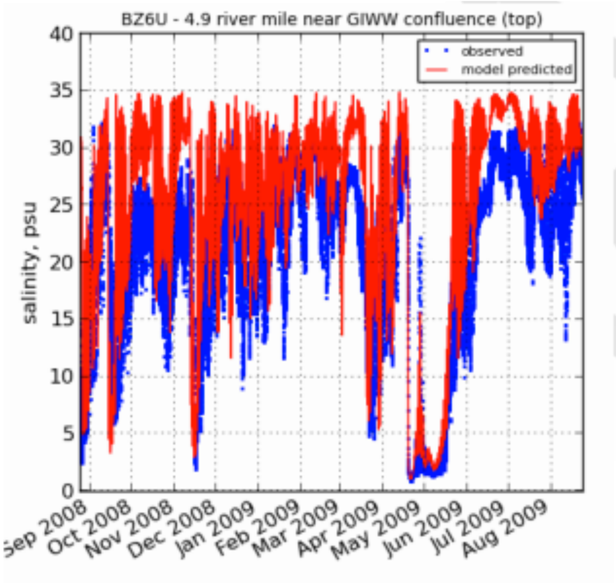


Figure 10. Salinity in BZ6U [3]

4.2 Additional test cases

Working with TWDB, we conducted a study using parameters described below, and using the second order TVD scheme for scalar transport at the wet/dry interface where element water depths go below .1m. We ran with a much smaller time step, 5 seconds vs. 90 seconds. We also tested various turbulence closure methods. What are presented below were judged to be the best solutions we were able to obtain.

4.2.1 Model Configuration

Table 6. Model configuration for second verification case

Model parameter	**Value used**
Model time step	5 seconds
Vertical resolution	15 sigma layers
Scalar transport scheme	2nd order TVD
Baroclinic/Barotropic flow	Baroclinic
Turbulence model and stability function	KE-GLS as k-epsilon; KC-Kantha & Clayson
Drag coefficient (Cd)	.0025 (Spatially uniform)
Maximum diffusivity	10-6 m2/s
Elements go dry at water depth	<0.1 m

4.2.2 Time series contour plots

In the time series contour plots depicted in this and subsequent sections, the X axis signifies the distance down the length of the river. X=0 is the furthest point on the grid depicting the head of the Brazos River, and X=46,000 m is at the mouth of the river, i.e.

where the river meets the Gulf of Mexico. The Z axis labels the 16 sigma layers used to quantify the depth of the river in the 3-D mesh used for these simulations.

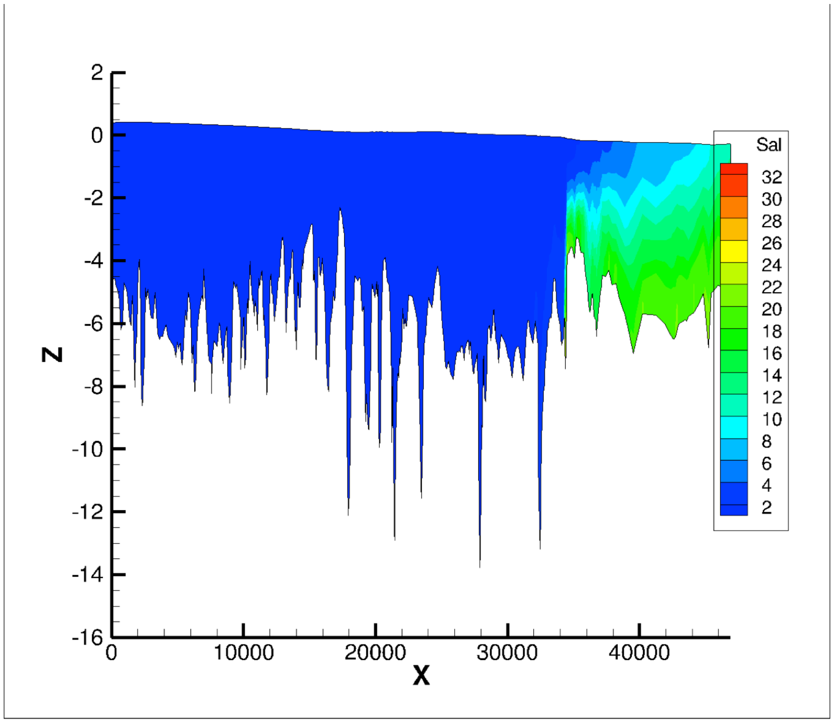


Figure 11. **t=13 days. Second verification case (units: X=meter, Z=level, Salinity=psu)**

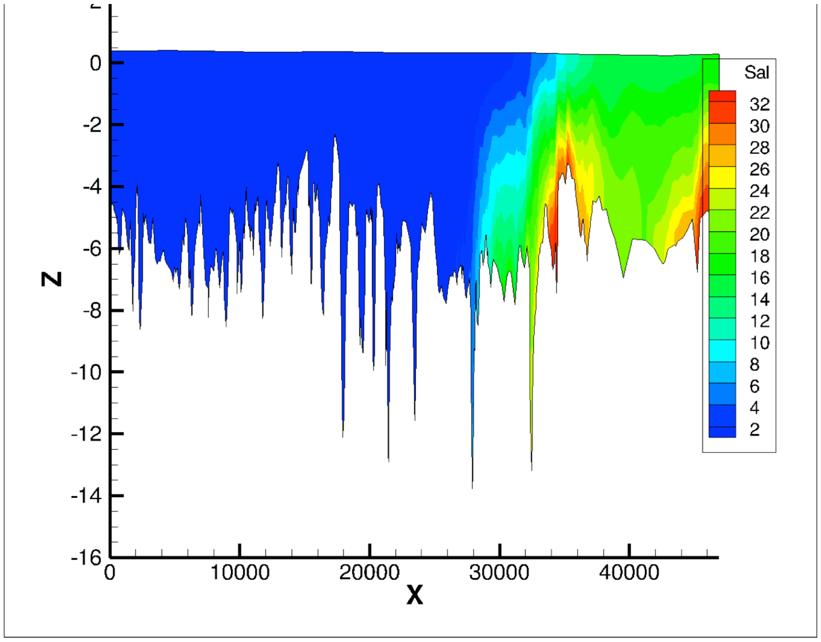


Figure 12. **t=26 days. Second verification case(units: X=meter, Z=level, Salinity=psu)**

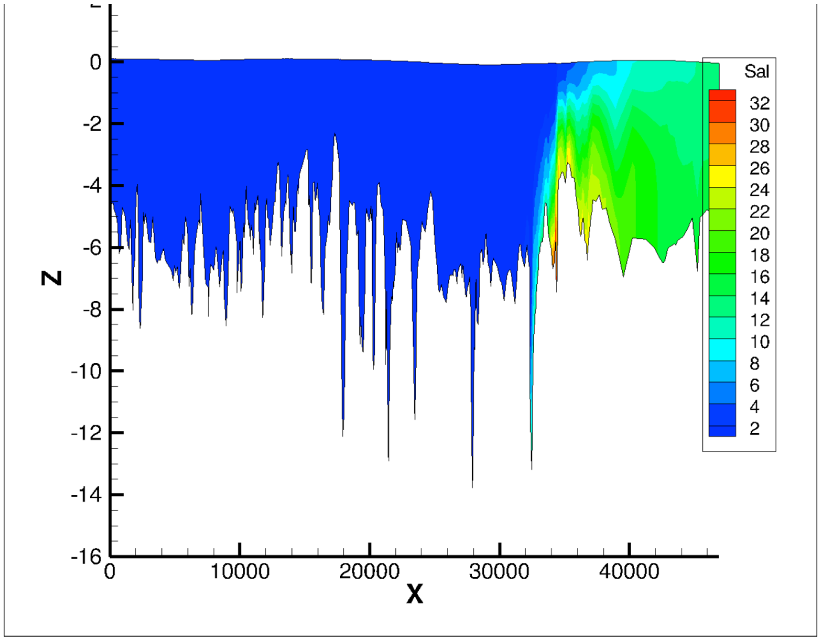


Figure 13. **t=38 days. Second verification case(units: X=meter, Z=level, Salinity=psu)**

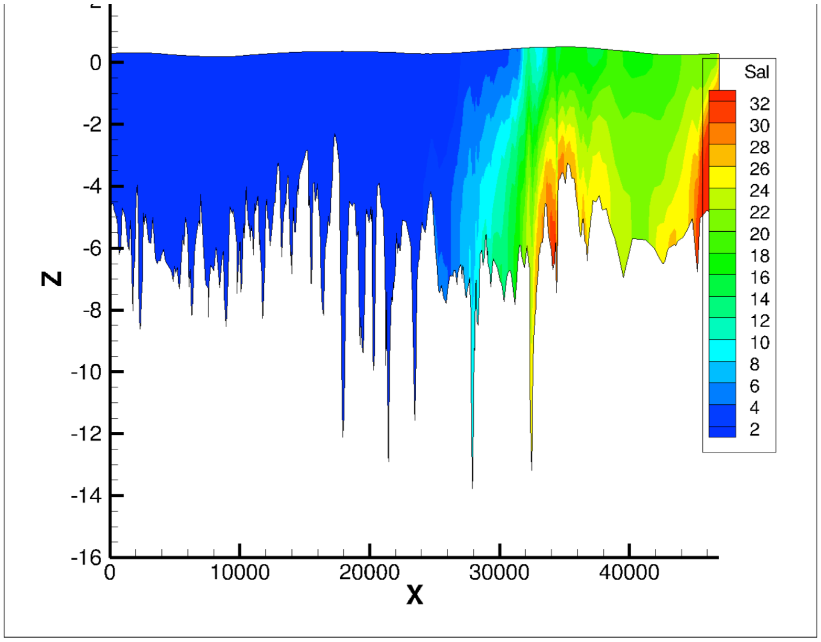


Figure 14. **t=50 days. Second verification case(units: X=meter, Z=level, Salinity=psu)**

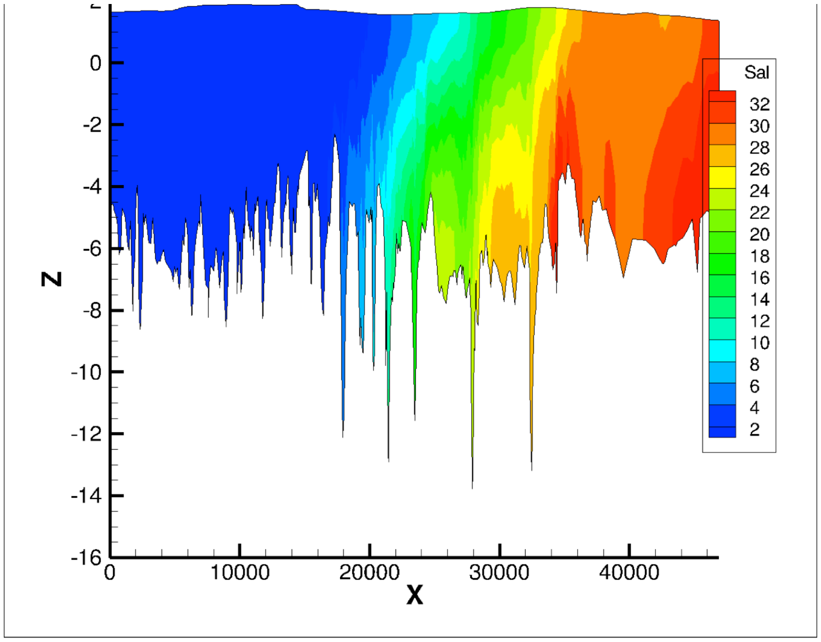


Figure 15. **t=63 days. Second verification case(units: X=meter, Z=level, Salinity=psu)**

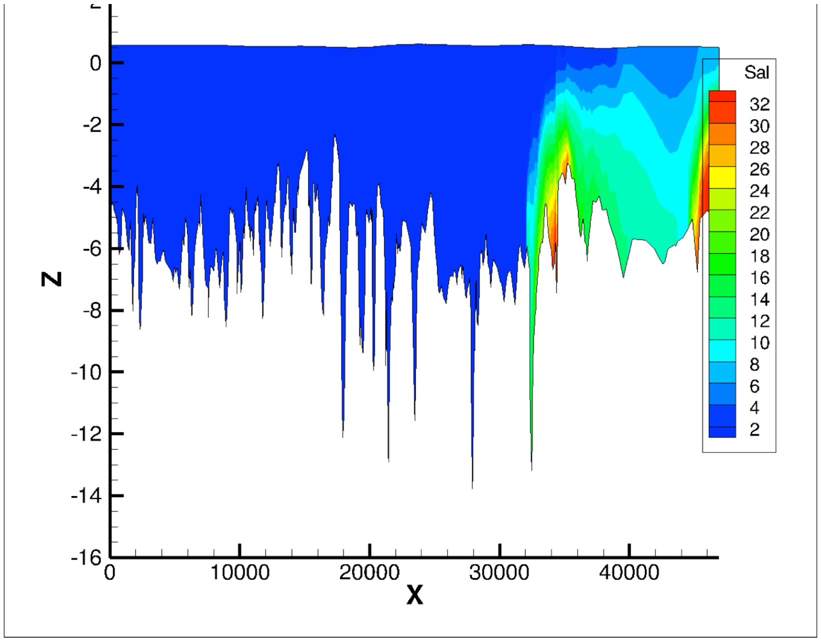


Figure 16. **t=76 days. Second verification case. (units: X=meter, Z=level, Salinity=psu)**

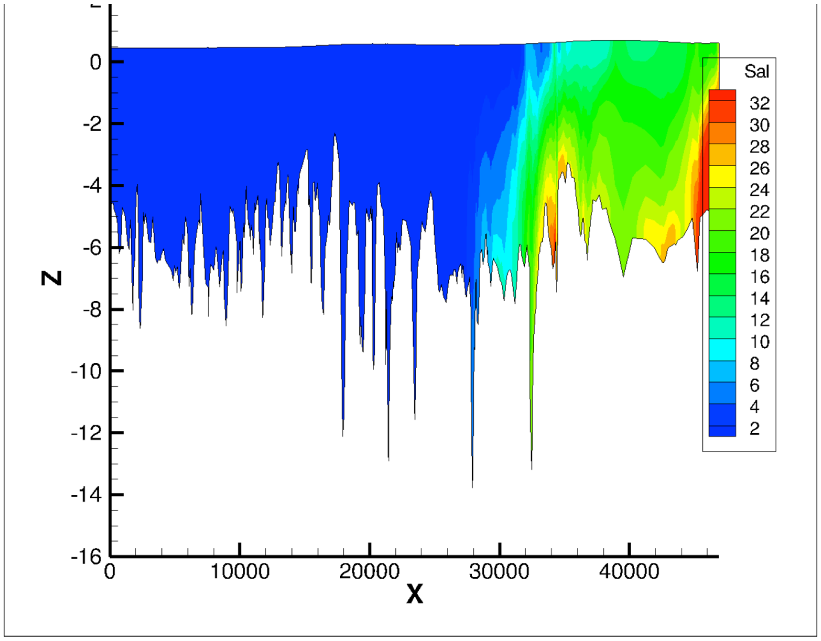


Figure 17. **t=90 days. Second verification case(units: X=meter, Z=level, Salinity=psu)**

The plots in Figures 11-17 show contours of salinity at various times over the course of 3 months. With the parameters set for this study described in the model configuration, we were able to generate results covering a span of 3 months in 24 hours of CPU time using 96 cores on the Stampede Supercomputer at the Texas Advanced Comptuting Center (TACC). As can be seen in the figures the salinity has some stratification issues throughout the time series. However, in discussion with TWDB this represents improvement from the previous studies conducted. The salt water is being pushed adequately into the river, and the freshwater into the ocean. So the majority of the interface issues faced earlier are now resolved through this study. To evaluate the improvements in the modeled results we compared it with the observed data, which we have plotted below. In this simulation, we have lowered the time-step and used a higher order transport scheme, but the grid remains the same as in the initial case.

4.2.3 Time History plots

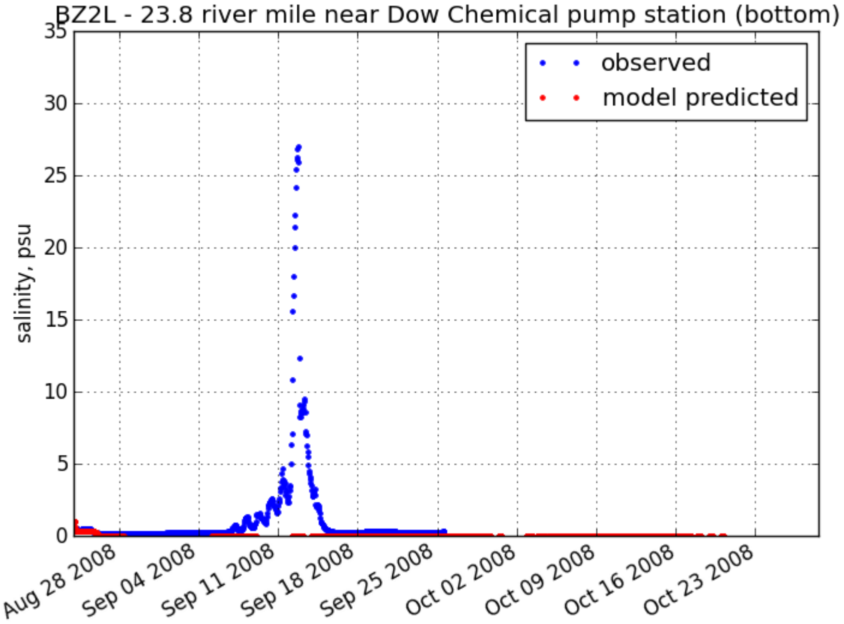


Figure 18. Salinities in bz2l

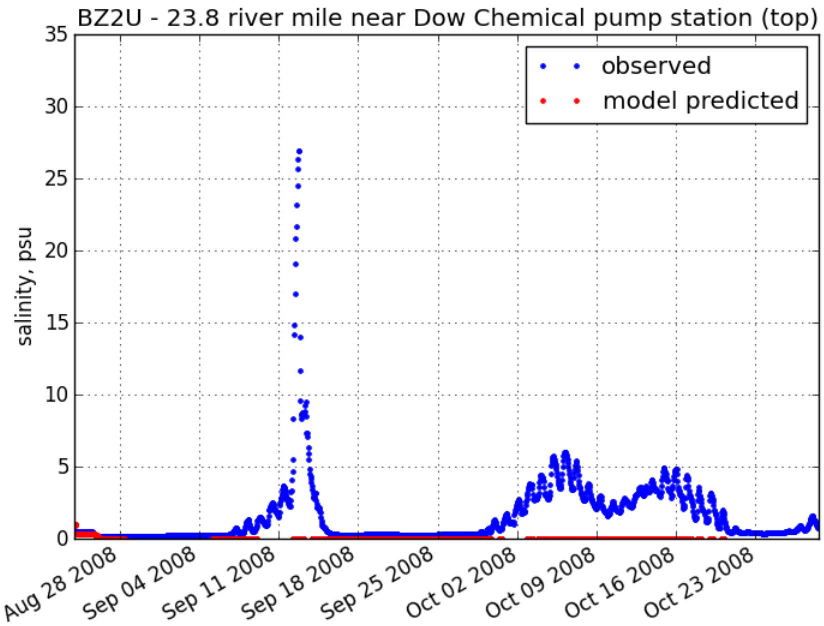


Figure 19. **Salinities in bz2u**

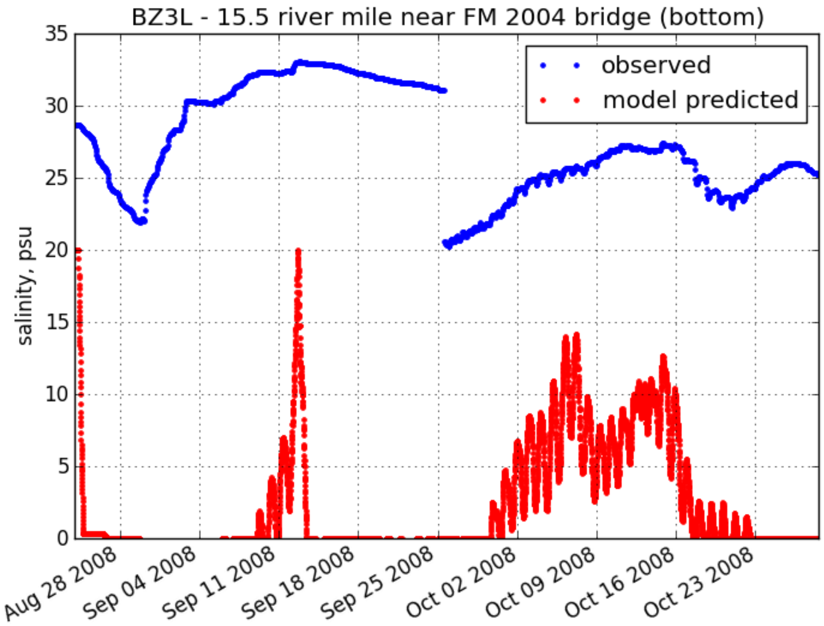


Figure 20. **Salinities in bz3l**

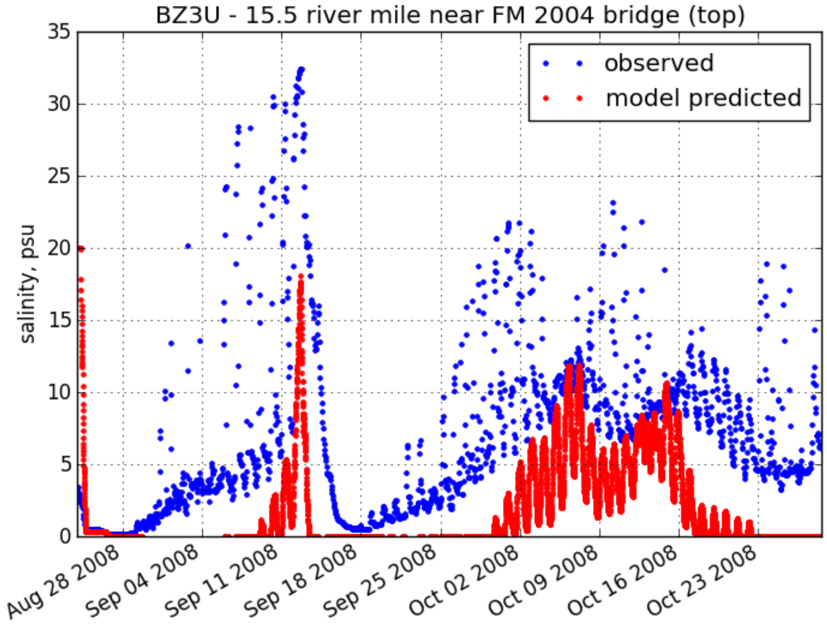


Figure 21. **Salinities in bz3u**

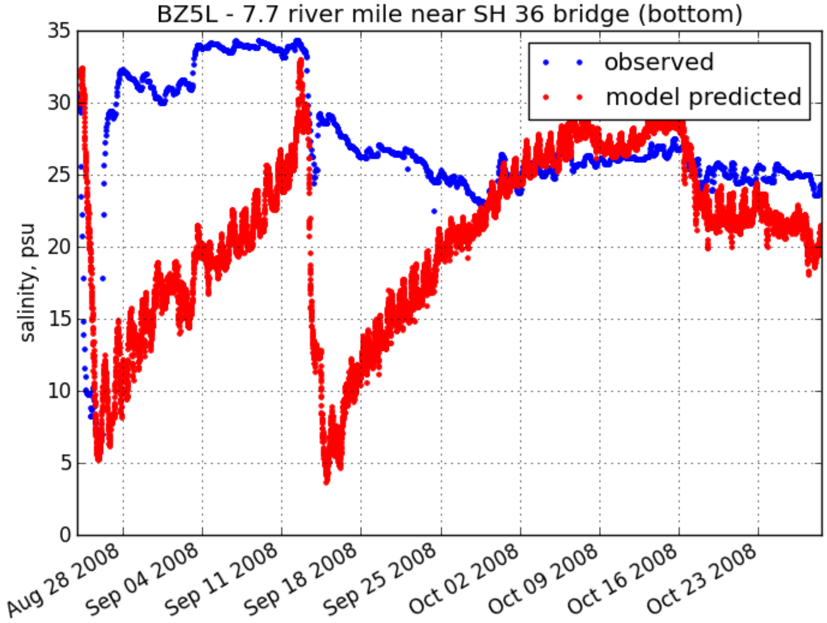


Figure 22. **Salinities in bz5l**

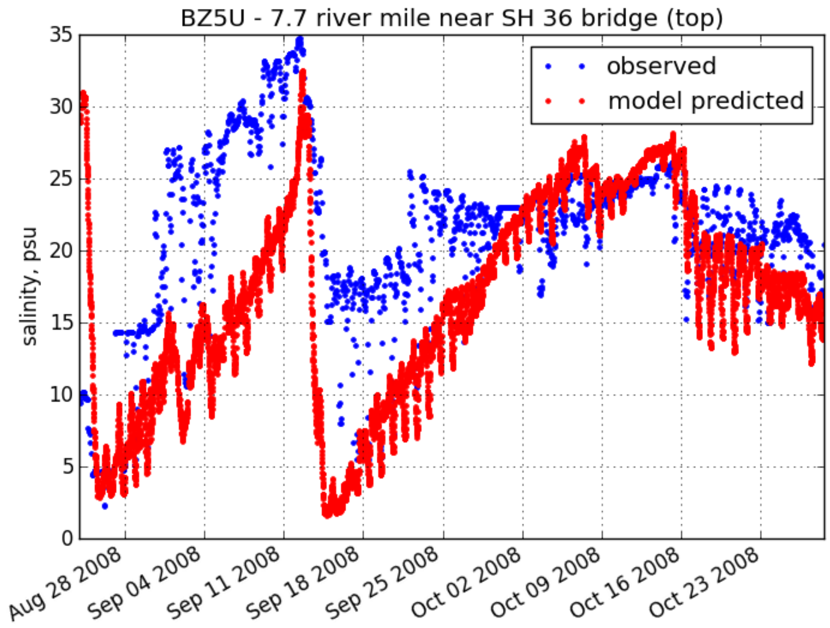


Figure 23. **Salinities in bz5u**

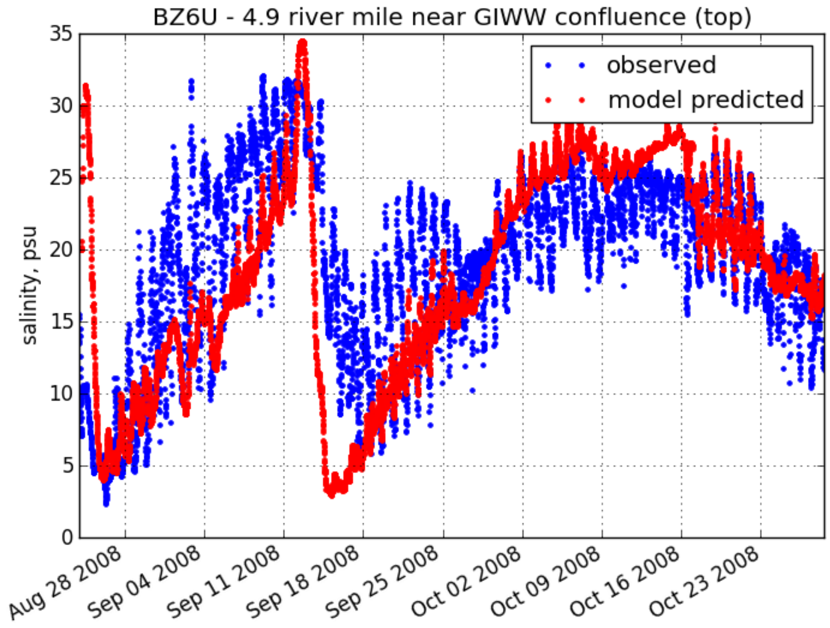


Figure 24. **Salinities in bz6u**

The time history plots in Figures 18-24 can be compared to Figures 6-10. There are still large discrepancies between model and data, especially in the stations that are further up the Brazos River. The stations closer to the Gulf, for example as shown in Figure 24, show fairly good agreement with the observations. Further up the river, for example, looking at station BZ3U for the month of October, we a see slightly closer match between observed and modeled results in this study compared to the initial one conducted by TWDB (Figure 8 vs. 21). Other results to compare would be Figure 24 vs. Figure 10, displaying results at station BZ6U. For the month of October, we see the highs of 35 ppt for salinity in Figure 10, but see a much closer match with salinity highs of 28 ppt in the Figure 24 with the observed results. Perhaps more importantly, we seem to obtain reasonable stratification in the river, as seen in Figures 11-17.

4.3 Refined Grid cases

4.3.1 Model Configuration

Table 7. Model configurations for refined grid case

Model parameter	**Value used**
Model time step	5 seconds
Vertical resolution	15 sigma layers
Scalar transport scheme	2nd order TVD- Casulli formulation
Baroclinic/Barotropic flow	Baroclinic
Turbulence model and stability function	0 – constant
Drag coefficient (Cd)	.0025 (Spatially uniform)
Maximum diffusivity	10-6 m2/s
Elements go dry at water depth	<0.1 m

We next performed simulations where we refined the grid by 2 standard levels. The new grid contained 153314 nodes and 291495 elements. We also used a slightly different 2nd order TVD method due to Casulli [7]. In addition we turned off the turbulence model since the particular form of the turbulence model did not seem to affect the results; i.e., we ran with zero diffusion. The results are presented in Figures 25-38. Unfortunately, the mesh refinement resulted in much slower execution. As can be seen in the figures we were only able to obtain about 5 days worth of results using 48 hours of CPU time on the TACC Stampede Supercomputer (the maximum time limit for any simulation). Clearly SELFE is not optimized for parallel computing, as it also does not scale with CPUs, therefore increasing the number of CPUs does not help with runtimes. This issue was beyond the scope of this project.

4.3.2 Time series contour plots

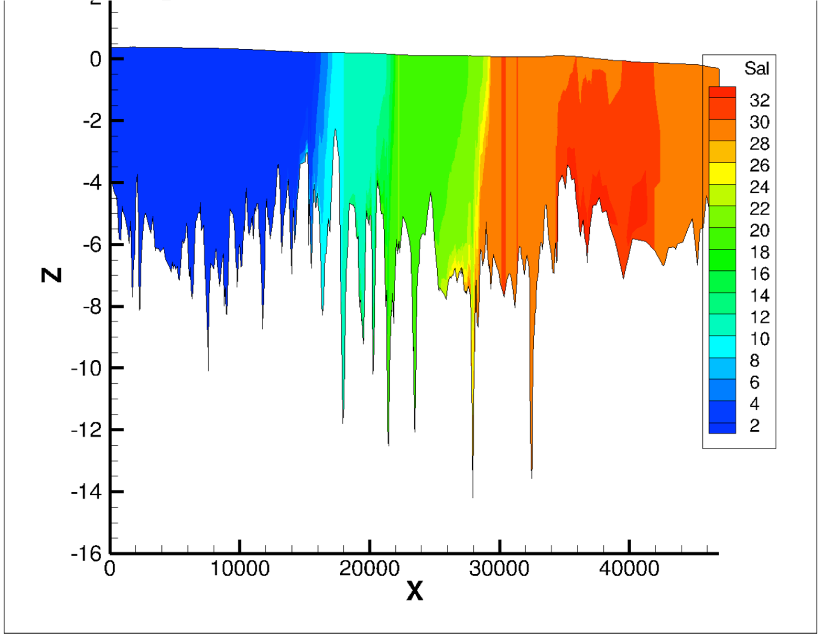


Figure 25. **t=0 days, refine grid case(units: X=meter, Z=level, Salinity=psu)**

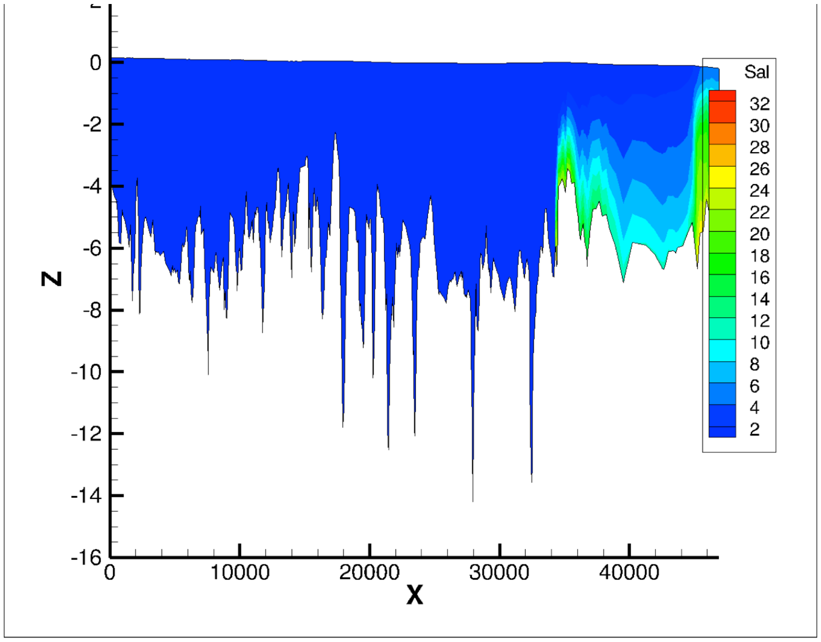


Figure 26. **t=1 day, refined grid case(units: X=meter, Z=level, Salinity=psu)**

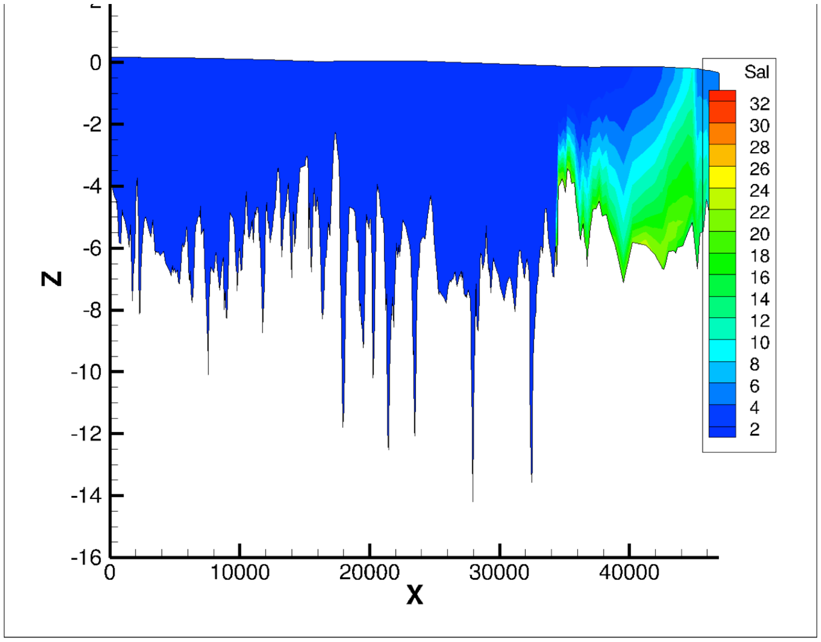


Figure 27. **t=2 days, refined grid case(units: X=meter, Z=level, Salinity=psu)**

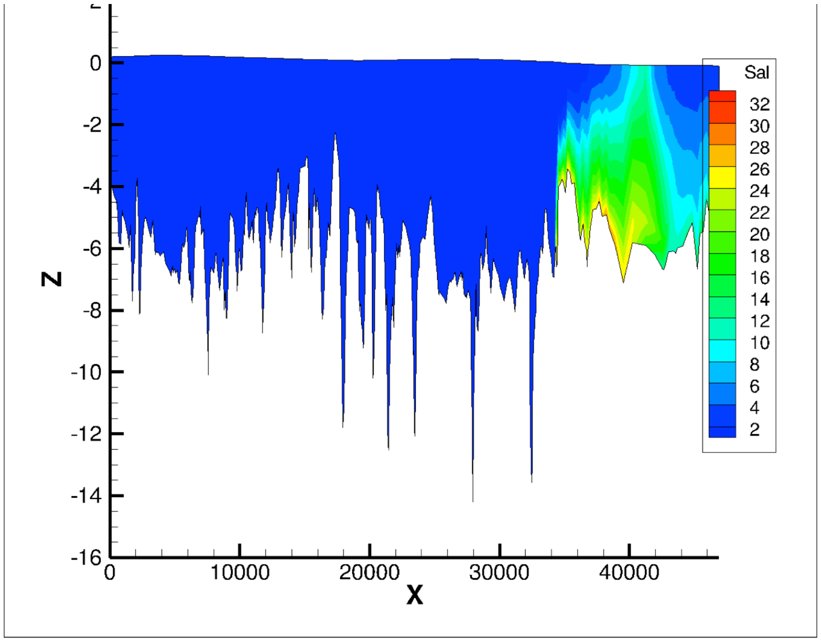


Figure 28. **t=3 days, refined grid case(units: X=meter, Z=level, Salinity=psu)**

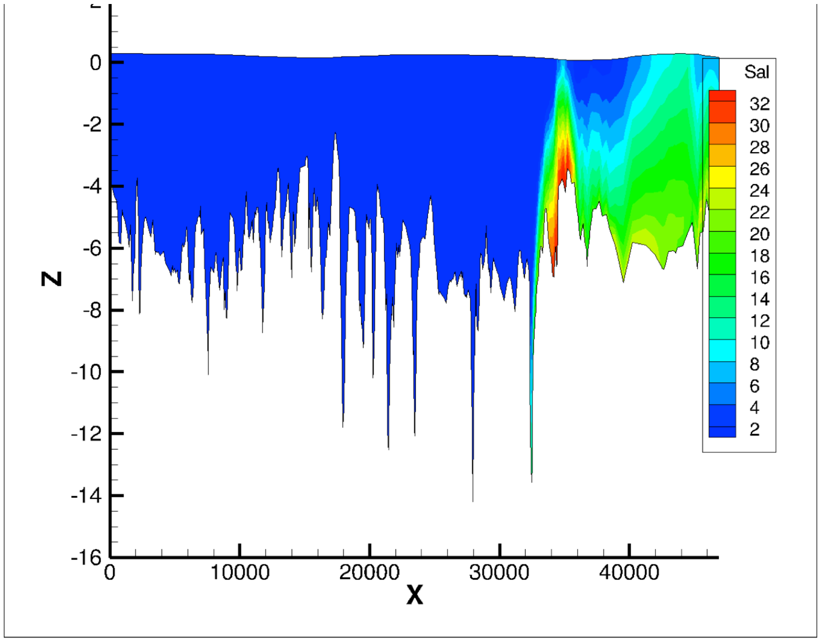


Figure 29. **t=4 days, refined grid case(units: X=meter, Z=level, Salinity=psu)**

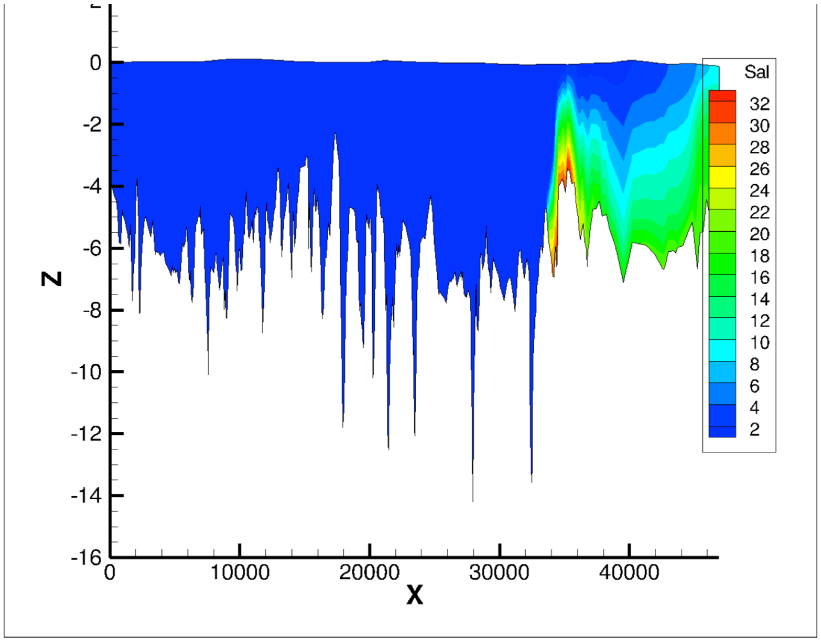


Figure 30. **t=5 days, refined grid case(units: X=meter, Z=level, Salinity=psu)**

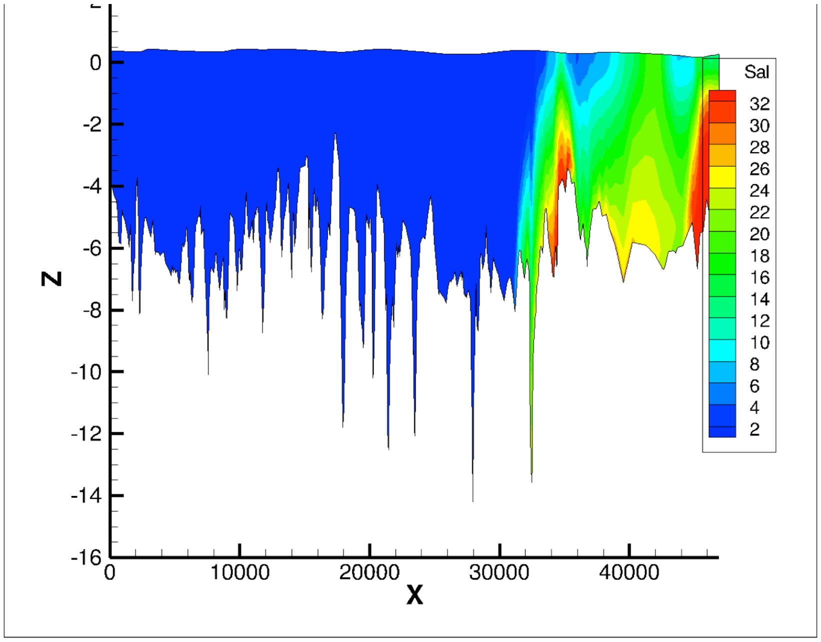


Figure 31. **t=5.5 days, refined grid case(units: X=meter, Z=level, Salinity=psu)**

We again see reasonable stratification in the refined grid case. The river is dominated by freshwater, with a mixing of fresh and salt water at the interface. These model parameters along with the refined grid reduce the numerical diffusion caused by the Eulerian-Lagrangian method (ELM) in SELFE for solving the Navier-stokes equations. Although the results may seem improved, it is hard to judge the true nature of trends since we were only able to obtain 5 days worth of results. Presented below are time-history plots for this simulation at the measurement locations.

4.3.3 Time history plots

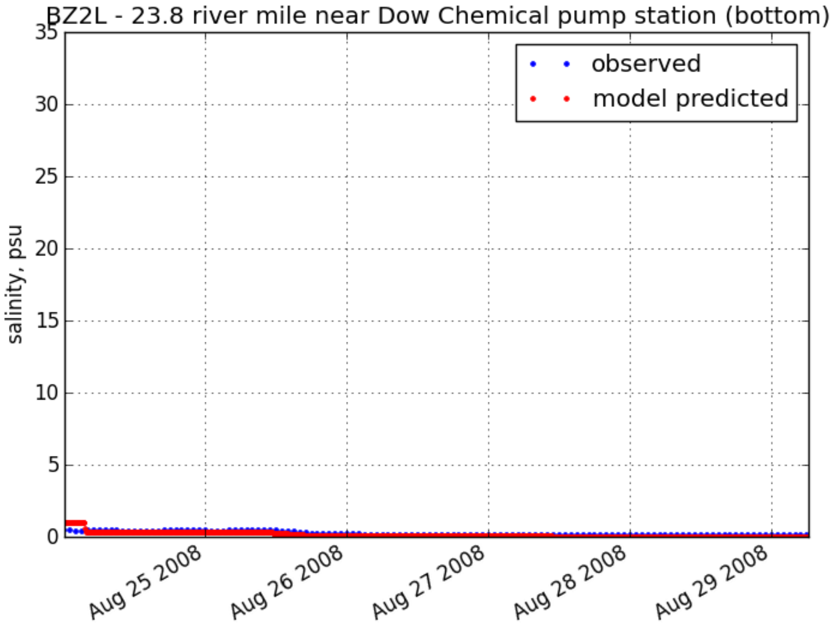


Figure 32. Salinities in bz2l

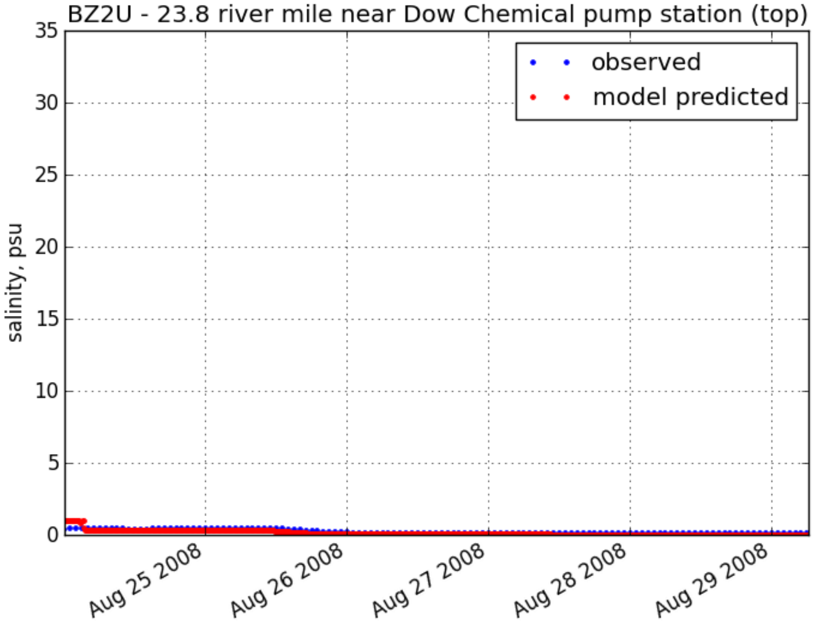


Figure 33. Salinities in bz2u

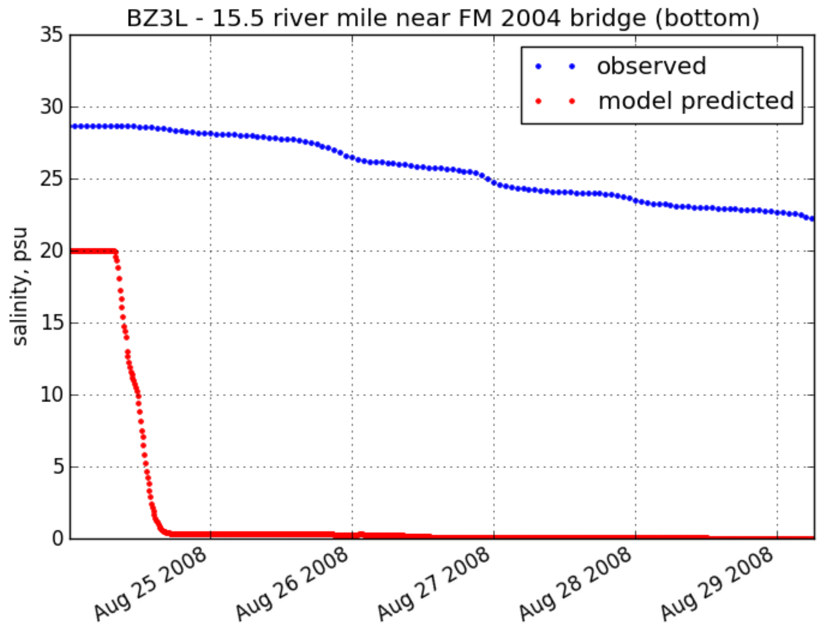


Figure 34. **Salinities in bz3l**

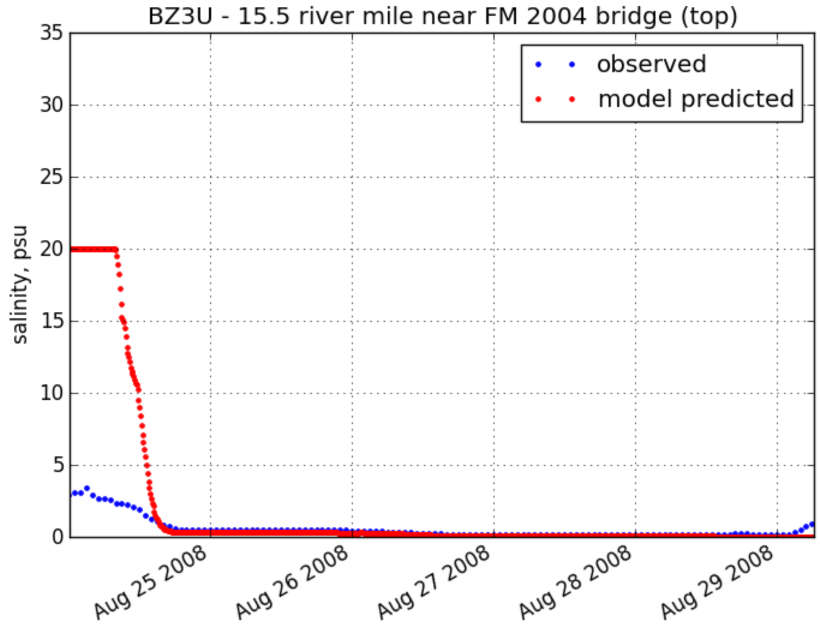


Figure 35. **Salinities in bz3u**

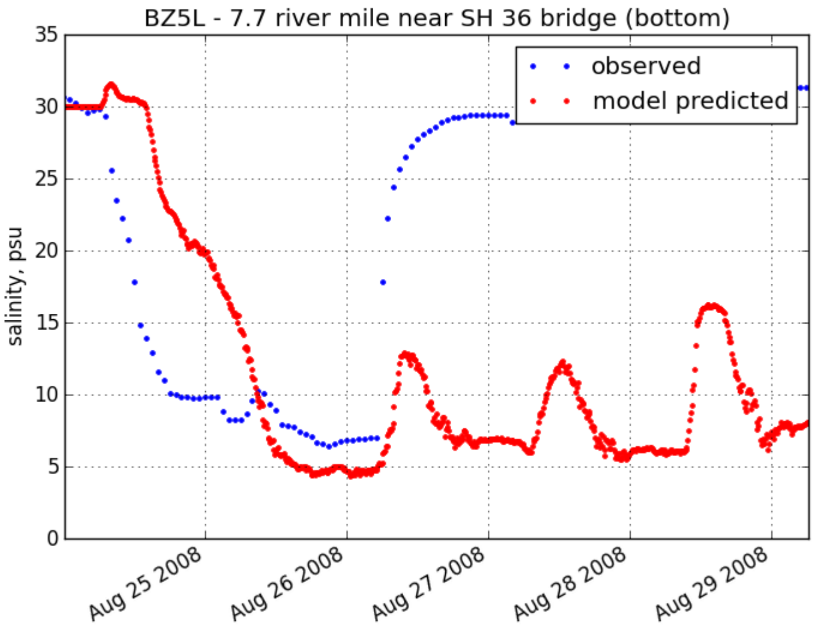


Figure 36. **Salinities in bz5l**

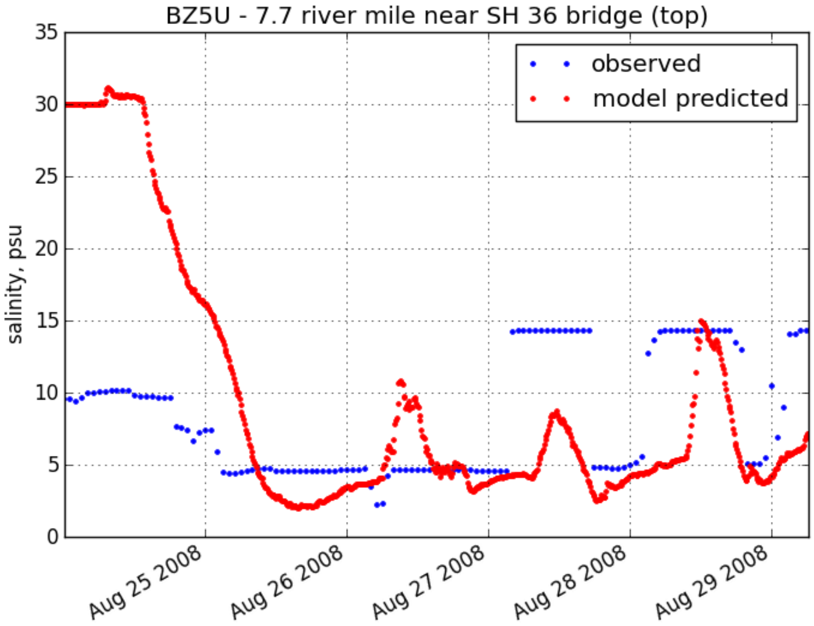


Figure 37. **Salinities at bz5u**

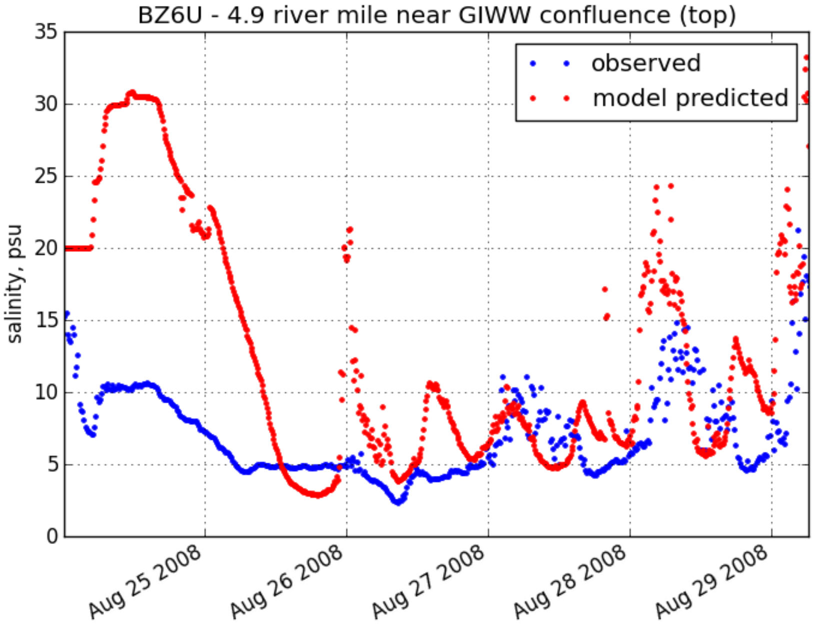
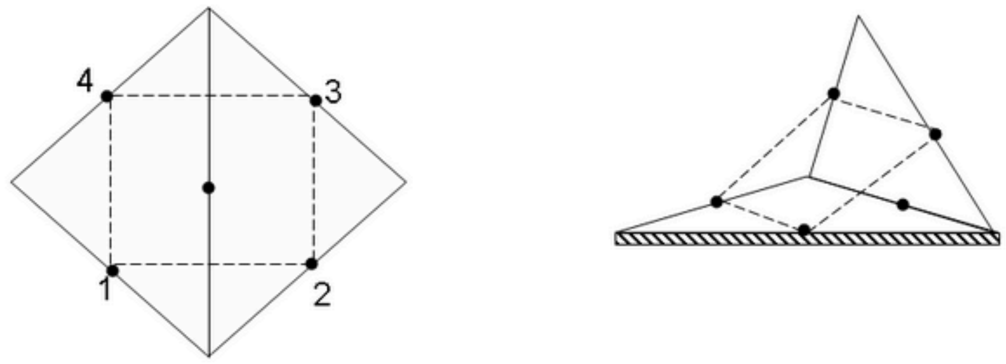


Figure 38. **Salinities at bz6u**

The refinement of the grid and the use of the Casulli formulation do seem to reduce numerical diffusion in the salinity stratification, however, the price is in the efficiency.

4.4 Updated “beta” version of SELFE

Towards the end of 2013, the latest beta version of SELFE was acquired from Joseph Zhang, the lead developer of SELFE, which will be referred to as “new selfe” in the figures below. This newer version of SELFE allows for the use of the 2nd order TVD transport method everywhere in the domain, with a Shapiro filter. However, as the code is in development, it was difficult to implement and there is little user support. After many efforts, this newer version of SELFE was compiled to run in parallel on the TACC super computer, Stampede. Several simulations were run during the past few months; however some issues were encountered. A major issue arises in the use of the Shapiro filter and constraints this places on the mesh. From the SELFE manual we read: “The use of a Shapiro filter (indvel=0 or -1) places some constraints on the boundary sides. In particular, the center of any internal sides must be inside the quad formed by the centers of its 4 adjacent sides. If not, the code will try to enlarge the stencil, but if the side is near the boundary, fatal error will occur. To find out all violating boundary elements, just prepare hgrid.gr3 (note that the open boundary info needs no be correct at this stage), vgrid.in and param.in up to ihorcon, and run the code with ipre=1 in param.in. You'll find a list of all such sides in fort.11 (the two node numbers of a side will be shown). Method to eliminate this problem includes: (1) move node, (2) swap the side for a pair of elements, and (3) refine or coarsen. Note that in most grid editors, the first 2 methods won't change the node numbering and so you'd try them first before Method (3), to save time. After the pre-processing run is successful (with a screen message indicating so), you can then proceed to prepare other inputs. If you use xmgredit5 (inside the ACE package), it can help you identify the elements/sides that need editing. Under the manual: Edit--> Edit over grid/regions --> Mark Shapiro filter violations, turn it on and you'll see some elements are highlighted. Not all those elements need to be edited - only those "pointing" outside the boundary [4]."



(a) The side center is inside the quad 1234.

(b) A typical boundary element with an obtuse angle facing the boundary, and a side center is *not* inside the quad.

Figure 39. Mesh requirements

We had to perform several iterations with the mesh before completely eliminating the mesh requirements. This was not a trivial task. In addition, we had issues compiling this version of SELFE , Jesse Thomas and Tomas Karna from Center for Coastal Margin Observation and Prediction helped with this process. Lastly, there were output issues. The station output files had ill-formatted output data that could not be organized and plotted. Therefore we could not obtain plots of model vs. observations. We will show the salinity contour plots below.

4.4.1 Salinity Contour plots from beta version of SELFE

The model configuration for this simulation was the same as the refined grid case defined above. The results up to 3.5 days of simulation are shown in Figures 40-46. The results at day 1 are similar to the previous run, comparing Figures 26 and 41. By day 3 however, the newer version of SELFE shows a quite different salinity profile near the mouth of the river (compare Figures 28 and 45). The possible reason for these differences is that the newer version uses a different implementation of the TVD method. In particular, the TVD transport scheme is now used everywhere in the domain rather than just in the shallow regions.

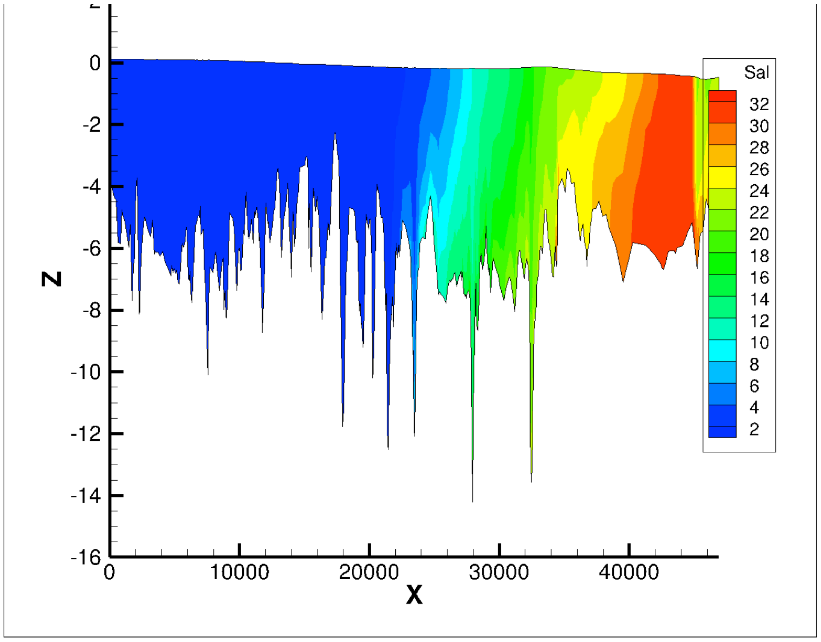


Figure 40. **New selfe: t=0.5 days (units: X=meter, Z=level, Salinity=psu)**

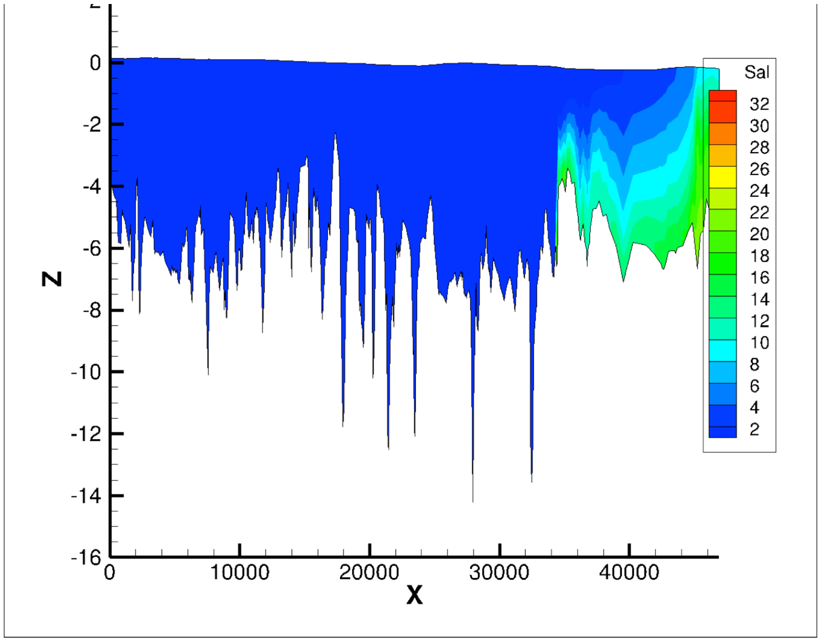


Figure 41. **New selfe t= 1 day (units: X=meter, Z=level, Salinity=psu)**

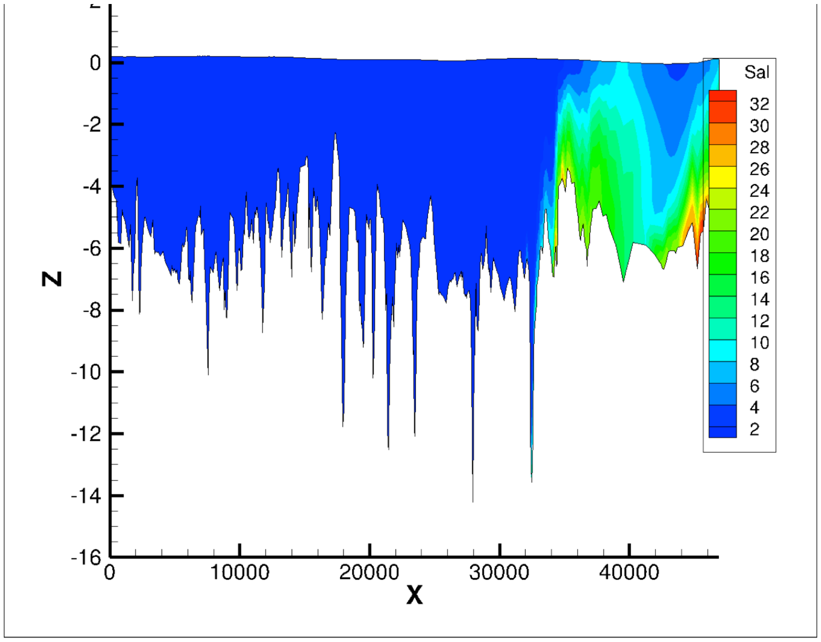


Figure 42. **New selfe t =1.5 days (units: X=meter, Z=level, Salinity=psu)**

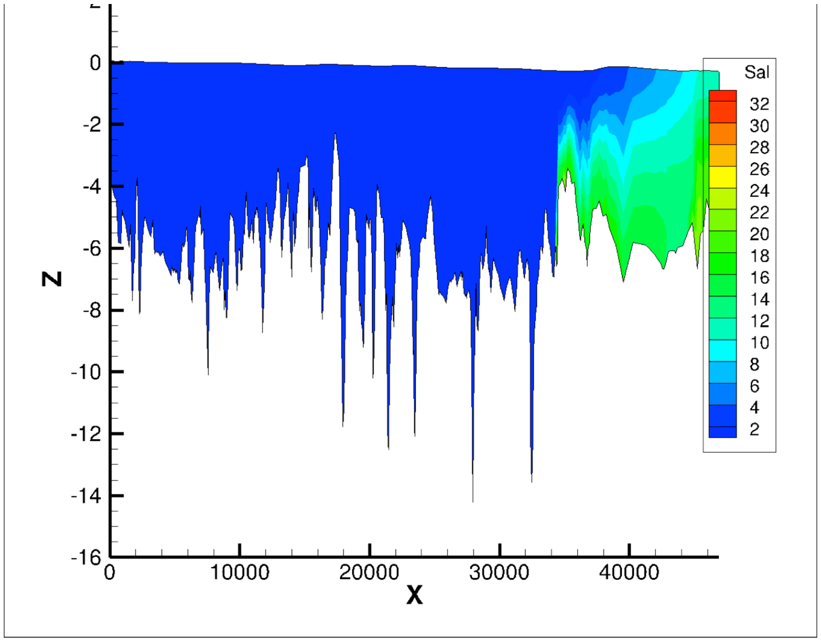


Figure 43. **New selfe t=2 days (units: X=meter, Z=level, Salinity=psu)**

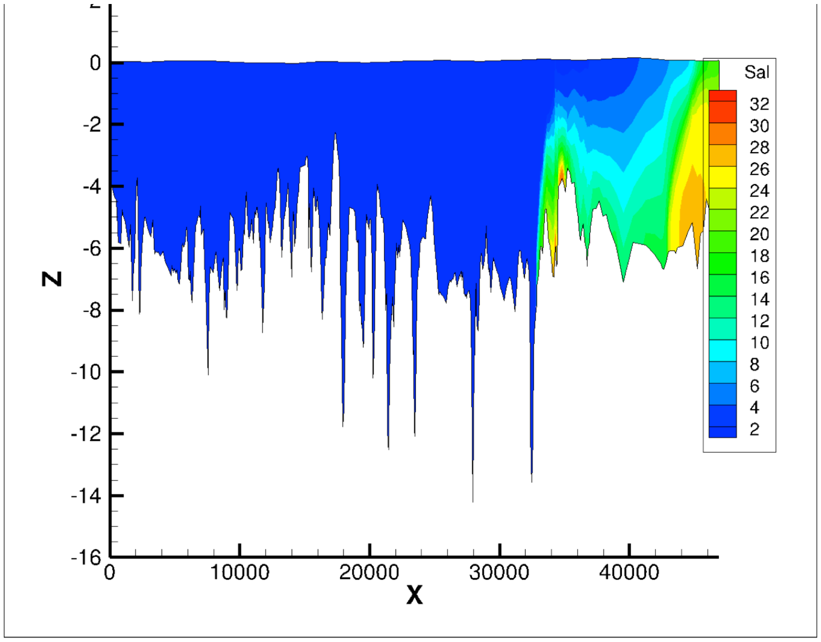


Figure 44. **New selfe t=2.5 days (units: X=meter, Z=level, Salinity=psu)**

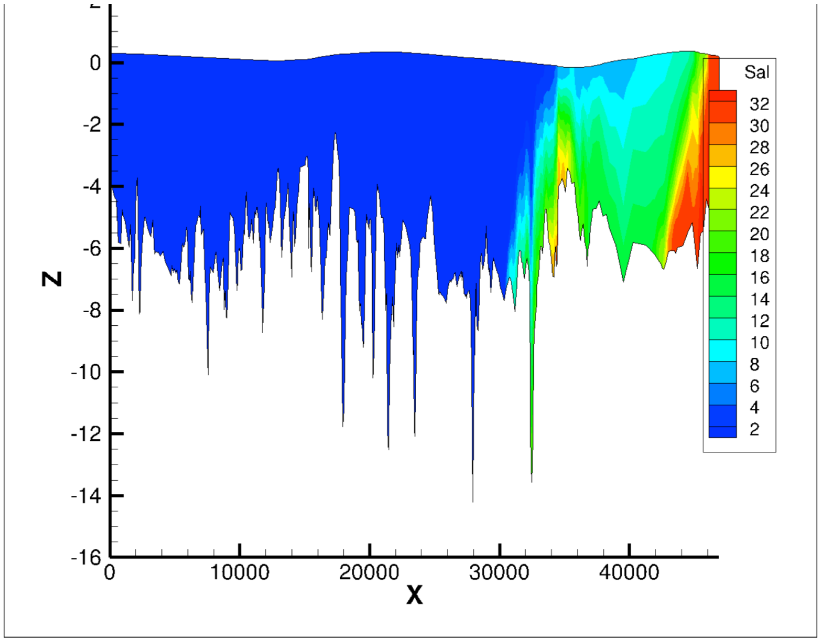


Figure 45. **New selfe t=3 days (units: X=meter, Z=level, Salinity=psu)**

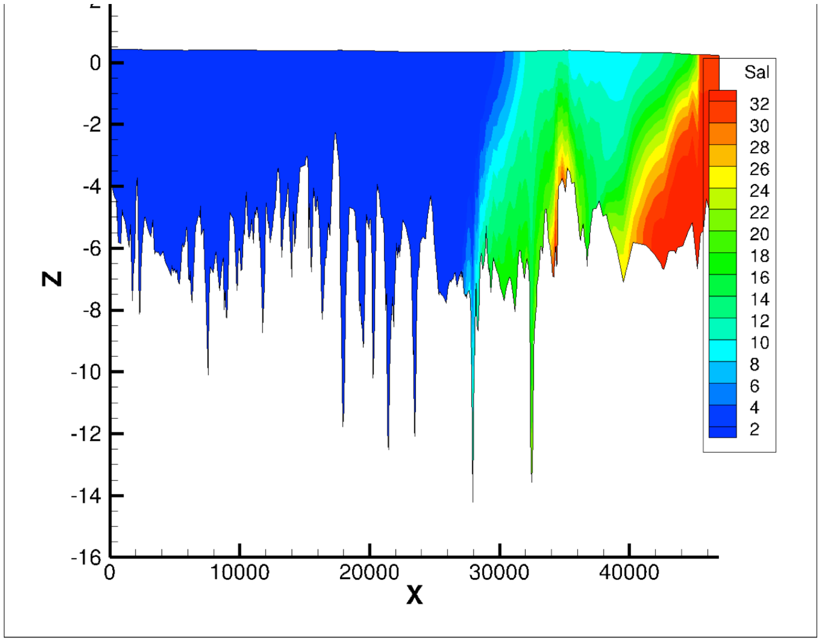


Figure 46. **New selfe t=3.5 days(units: X=meter, Z=level, Salinity=psu)**

4 Conclusions and recommendations

The use of higher order TVD transport schemes in SELFE along with refined mesh and smaller time-steps seems to improve the salt-water/fresh water interface in the Brazos River area. The updated version of SELFE did provide better numerical stability of the solution but the improvement was not significant enough to provide improved comparisons with measured data.

In summary, we make the following observations on the use of higher order TVD transport methods, along with refined mesh and smaller time steps:

1) Improvement in stratification. We see physically reasonable results in the freshwater/saltwater interface throughout most of the domain and throughout the time period of the simulation.

2) Due to the cyclic nature of the results, it is safe to speculate that the quarter year simulations in Figures 18-24 are a good representative of the year. We see for example in BZ3U (Figure 21) using the second order TVD scheme and smaller time step gives a slightly closer match between model and observations than in Figure 8 where a first order upwind scheme was used along with a larger time step. The difference between high and low points is approximately 20 psu, however in the improved Figure 21, we see that difference to be 5 psu. We see similar improvements in other stations such as BZ2L and BZ2U, where the average trends between observation and model are in fairly good agreement.

We have tested grid refinement, time-step refinement, different turbulence and transport schemes. We did not modify the 3-D shallow water Eulerian-Lagrangian solver in SELFE. The main concern going forward with SELFE is in the Eulerian-Lagrangian method for solving the 3-D shallow water equations and numerous restrictions that it carries with it. The developers of SELFE themselves have said that this method is numerically diffusive, but cannot be changed without rewriting the software in it's entirety.

5 Appendices

Appendix A: User instructions for conducting salinity studies using SELFE

For all the file samples, please refer to the SELFE manual [4].

1) The parameters are set in param.in file.
2) The boundary conditions in bctides.in
3) A horizontal grid file, and a vertical grid file with sigma levels must be provided.
4) The new version of SELFE requires tvd.prop file to specify on what elements to implement the TVD scheme.
5) Time history files for flux, elevation and salinity are required if boundaries are not specified a constant value.
6) Files for minimum and maximum diffusivity on nodes are required if constant values are not used.
7) A file containing station locations must be specified for station outputs
8) File drag.gr3 must be specified with drag coefficient at each node.
9) If source or sink for salinities are introduced then an input file with node numbers for sinks and sources must be used while running the code.
10) An output directory must be specified within the running folder, where all the results will be outputted.
11) Run the executable by submitting it via que on stampede or any cluster.

5.2 Appendix B: User instructions for Post-processing

1) Direct the perl script autocombine.pl to the ouput directory. The out files of concern will be of two types- global and local.
2) The local files needs to be combined. The global files can be used for visualization.

Local files:

The local files will be of format- recorded time period__processor#__attribute.*, where recorded time period is the intervals of data recorded from each set of time interval of total simulation. For example, every day, or every hour- however often and amount of data to record in a file before moving on to the next time period.

The processor # is the processor from which the data is collected. It depends on the cluster size, and user specification of the number of processors to use.

The attributes are salinity, horizontal velocity, elevation, flux or numerous other choices which the user can specify in param.in. and the star refers to .63, 64 numbers for labeling purposes only.

3) The autocombine script will combine the outputs from different processors into single, and the resulting global files will be of format recorded time interval__attribute.*
4) Some of the other global outputs are staout_* where staout is station output, and * refers to the attribute.

5.3 Appendix C: User instructions for visualization

The visualization scripts are very simple to use. These scripts have been delivered to TWDB along with this report. The basis of these scripts was derived from scripts written by Solomon Negusse of TWDB.

1) The global salinity files from each recorded time period can be combined into a dat file which can then be converted to plt file using tecplot's preplot utility.
2) This plt file can then be visualized using tecplot.
3) The station output files can be visualized using python script for plots of recorded vs modeled salinity, say. This requires an input file with recorded data at the stations.

6 References

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http://www.stccmop.org/knowledge_transfer/software/selfe

[2] TWDB Scope of Work. Exhibit A. Clint Dawson.

[3] Negusse, Solomon. Influences of the Lower Brazos River Realignment and Construction of the Gulf Intracoastal Waterway on the Brazos River and the San Bernard River Estuaries. May 2014.
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[5] Zhang Y, Baptista AM. 2008. SELFE: A semi-implicit Eulerian–Lagrangian finite-element model for cross-scale ocean circulation. Ocean Modelling. 21(3-4):71-96.

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