Discontinuous Galerkin discretization for two-equation turbulence closure model

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Abstract
Accurate representation of vertical turbulence is crucial for numerical ocean modelling, both in global and coastal applications. The state-of-the-art approach is to use two-equation turbulence closure models which introduces two dynamic equations to the system. Solving these equations numerically, however, is challenging due to the strict requirement of positivity of the turbulent quantities (e.g. turbulence kinetic energy and its dissipation rate), and the non-linear source terms that may render the numerical system unstable. In this paper, we present a Discontinuous Galerkin (DG) finite element discretization of the Generic Length Scale equations designed to be incorporated within a DG coastal ocean model. We validate the implementation with standard turbulence closure model benchmarks and an idealized estuary simulation. Finally, we use the full three-dimensional model to simulate the Columbia River plume. The results confirm that the coupled model generates realistic vertical mixing, and remains stable under strongly stratified, energetic conditions. Estuarine circulation and river plume characteristics are well captured. Overall, numerical mixing of the model is found to be small resulting in a highly dynamic river plume.

Keywords: Oceanic turbulence, Turbulence closure models, Finite element method, Discontinuous Galerkin method, Estuarine dynamics, River plumes
1. Introduction

Ocean models usually rely on parametrizations to account for sub-grid scale vertical mixing processes. The relevant eddy coefficients are obtained by the means of turbulence closure models. While in some applications simple parametrizations, such as algebraic expressions of eddy viscosity and diffusivity, can be sufficient, in general more sophisticated schemes are needed in order to model the space-time evolution of the turbulent fields.

Representing the dynamic evolution of turbulent fields is crucial especially in coastal, buoyancy-driven applications. Vertical mixing plays a major role in the evolution of stratification and formation of the surface mixed layer. It is also essential in estuarine circulation, which in general cannot be simulated without a sophisticated turbulence closure model. Evolution of frontal features, such as in river plumes, is another example where algebraic parametrizations are not sufficient.

In ocean modeling, the most popular turbulence closures are two-equation models. These models consist of two partial differential equations, one for the turbulent kinetic energy (TKE), and another one for an accompanying variable that defines the turbulent length scale. Such models include the Mellor-Yamada (level 2.5) model (Mellor and Yamada, 1982), $k - \varepsilon$ (Rodi, 1987), $k - \omega$ model (Wilcox, 1988), and the Generic Length Scale (GLS; Umlauf and Burchard, 2003) model. The benefit of the GLS formulation is that all of the above closures can be obtained merely by changing parameters.

The turbulent eddy viscosity and diffusivity are obtained from the state variables, scaled by so-called non-dimensional stability functions. Most common stability functions are full-equilibrium functions by Canuto et al. (2001) (Canuto A and B), and by Cheng et al. (2002). Quasi-equilibrium functions, such as by (Kantha and Clayson, 1994), are also often used but have shown to be of limited applicability (Umlauf and Burchard, 2005).

Many existing ocean models implement two-equation turbulence closure models. The generic GLS model has become popular in recent years; it has been implemented in SELFE (Zhang and Baptista, 2008), SCHISM (Zhang et al., 2016), ROMS (Shchepetkin and McWilliams, 2003; Warner et al., 2005) and NEMO (Gurvan et al., 2017), for example, in addition to its original implementation in GOTM (Burchard et al., 1999).

In this paper, we present a finite element discretization of the GLS equations intended to be incorporated in a Discontinuous Galerkin (DG) three-dimensional circulation model. We present the weak formulation of the gov-
erning equations and a positivity preserving, semi-implicit time integration scheme. The model is implemented in the Thetis ocean model [Kärnä et al., 2018].

The GLS equations and stability functions are presented in Section 2. The principle of positivity preserving time discretization is outlined in Section 2.6. The finite element discretization and time integration scheme is presented in Section 3. Test cases are presented in Section 4, including a realistic application to the Columbia River plume in Section 4.4, followed by Discussion and Conclusions in Sections 5 and 6.

2. Two equation turbulence closure models

2.1. Generic Length Scale equations

The Generic Length Scale turbulence closure model [Umlauf and Burcharld, 2003] solves the two equations for turbulent kinetic energy (TKE), $k$, and an associated length scale, $\Psi$:

$$\frac{\partial k}{\partial t} + \nabla_h \cdot (ku) + \frac{\partial (wk)}{\partial z} = \frac{\partial}{\partial z} \left( \frac{\nu}{\sigma_k} \frac{\partial k}{\partial z} \right) + P + B - \varepsilon, \quad (1)$$

$$\frac{\partial \Psi}{\partial t} + \nabla_h \cdot (u\Psi) + \frac{\partial (w\Psi)}{\partial z} = \frac{\partial}{\partial z} \left( \frac{\nu}{\sigma_\Psi} \frac{\partial \Psi}{\partial z} \right) + \frac{\Psi}{k} \left( c_1 P + c_3 B - c_2 \varepsilon \right), \quad (2)$$

where $\sigma_k$ and $\sigma_\Psi$ are the Schmidt numbers for the two state variables, respectively.

The source terms in (1) are production of TKE, $P$; buoyancy production, $B$; and TKE dissipation rate $\varepsilon$. $P$ and $B$ depend on the vertical shear frequency $M$ and buoyancy (Brunt–Väisälä) frequency $N$:

$$P = \nu M^2, \quad (3)$$

$$B = -\nu' N^2, \quad (4)$$

$$M^2 = \left( \frac{\partial u}{\partial z} \right)^2 + \left( \frac{\partial v}{\partial z} \right)^2, \quad (5)$$

$$N^2 = -\frac{g}{\rho_0} \frac{\partial \rho}{\partial z}, \quad (6)$$

where $g$ is the gravitational acceleration, $\rho$ is the density of the water, and $\rho_0$ denotes a constant reference density.
The auxiliary length scale, $\Psi$, is defined by the parameters $p, m, n$:

$$\Psi = (c_\mu^0)^p k^m l^n,$$

where $c_\mu^0$ is an empirical parameter, and $l$ is a turbulent length scale. The TKE dissipation rate, $\varepsilon$, and turbulent length scale, $l$, are computed diagnostically from the state variables:

$$\varepsilon = (c_\mu^0)^{3+p/n} k^{3/2+m/n} \Psi^{-1/n},$$

$$l = (c_\mu^0)^{3+p/n} k^{-m/n} \Psi^{1/n}.$$

Based on (8) it is clear that choosing $p = 3, m = 3/2, n = -1$ results in the $k - \varepsilon$ model [Rodi, 1987].

The eddy viscosity and diffusivity are given by

$$\nu = c_\mu k^2 / \varepsilon,$$

$$\nu' = c'_\mu k^2 / \varepsilon,$$

respectively, where $c_\mu, c'_\mu$ are stability functions that depend on $N^2$ and $M^2$.

In the system (1-2), the empirical parameters $c_1, c_2$ and $c_3$ depend on the closure and the chosen stability functions.

The parameter $c_3$ controls buoyancy production of $\Psi$. It is split to two different values for stable and unstable stratification, respectively:

$$c_3 = \begin{cases} c_3^-, & \forall N^2 \geq 0 \\ c_3^+, & \forall N^2 < 0 \end{cases}$$

The parameter $c_3^+$ is used to control mixing in unstably stratified conditions; for the closures considered herein $c_3^+ = 1.0$.

2.1.1. Boundary conditions

Boundary conditions at the surface and bottom boundaries can be derived by assuming the law-of-the-wall boundary layer. With this assumption, the turbulent length scale grows linearly with the distance from the boundary, i.e.
\[ l_s = \kappa((\eta - z) + z_{0,s}), \]  
\[ l_b = \kappa((h + z) + z_{0,b}), \]  
respectively. Above \( z_{0,s}, z_{0,b} \) are the corresponding roughness length scales, \( \eta \) is the free surface elevation and \( h \) the bathymetry. TKE in the boundary layer is [Burchard et al. 1999]:

\[ k_s = \frac{(u^*_s)^2}{(c_0^s)^2}, \]  
\[ k_b = \frac{(u^*_b)^2}{(c_0^b)^2}, \]

where \( u^*_s \) and \( u^*_b \) are the friction velocities. From (15)-(16) the Neumann condition for \( k \) can be derived:

\[ \left. \frac{\nu}{\sigma_k} \frac{\partial k}{\partial z} \right|_{\Gamma_s} = 0 \]  
\[ \left. \frac{\nu}{\sigma_k} \frac{\partial k}{\partial z} \right|_{\Gamma_b} = n \frac{\nu}{\sigma_k} k m \kappa^n \left( \frac{\Delta z}{2} + z_{0,b} \right)^n. \]

In practice the gradients cannot be evaluated right at the boundary, and one typically sets \( (\eta - z) = (h + z) = \gamma \Delta z \), where \( \Delta z \) is the vertical element size, and \( \gamma > 0 \). The the parameter \( \gamma \) must be consistent with the bottom stress formulation of the mean flow model. Here value \( \gamma = 1/2 \) is used. The \( \Psi \) boundary conditions then become

\[ \left. \frac{\nu}{\sigma_\Psi} \frac{\partial \Psi}{\partial z} \right|_{\Gamma_s} = -n \frac{\nu}{\sigma_\Psi} (c_0^s)^p k^m \kappa^n (\Delta z/2 + z_{0,s})^{n-1} \]  
\[ \left. \frac{\nu}{\sigma_\Psi} \frac{\partial \Psi}{\partial z} \right|_{\Gamma_b} = n \frac{\nu}{\sigma_\Psi} (c_0^b)^p k^m \kappa^n (\Delta z/2 + z_{0,b})^{n-1}. \]
2.2. Steady state solution

In steady state, the source terms of the governing equations cancel out resulting in

\[ P + B - \varepsilon = 0 \]  \hspace{1cm} \text{(24)}
\[ c_1 P + c_3 B - c_2 \varepsilon = 0 \]  \hspace{1cm} \text{(25)}

It is convenient to define non-dimensional shear and buoyancy frequencies (Burchard and Bolding, 2001),

\[ \alpha_M = \frac{k^2}{\varepsilon^2} M^2, \]  \hspace{1cm} \text{(26)}
\[ \alpha_N = \frac{k^2}{\varepsilon^2} N^2. \]  \hspace{1cm} \text{(27)}

Using the gradient Richardson number,

\[ R_i = \frac{N^2}{M^2} = \frac{\alpha_N}{\alpha_M}, \]  \hspace{1cm} \text{(28)}

the equilibrium condition (24)-(25) can be expressed as (Umlauf and Burchard, 2003)

\[ R_i^{st} = \frac{c_\mu(R_i^{st})}{c'_\mu(R_i^{st})} \frac{c_2 - c_1}{c_2 - c_3}, \]  \hspace{1cm} \text{(29)}

where \( c_\mu \) and \( c'_\mu \) are the stability functions, and \( R_i^{st} \approx 1/4 \) denotes the steady state gradient Richardson number.

The steady state condition (24) can also be written as (eq 49 Umlauf and Burchard, 2005)

\[ c_\mu \alpha_M - c'_\mu \alpha_N = 1. \]  \hspace{1cm} \text{(30)}

From (30) and (28) it follows that in equilibrium the stability functions only depend on \( R_i^{st} \): \( c_\mu = c_\mu(R_i^{st}) \), \( c'_\mu = c'_\mu(R_i^{st}) \).
2.3. Length scale limitation

Galperin et al. (1988) suggested to limit $l$ as

$$l \leq l_{\text{max}} = c_{\text{lim}} \frac{\sqrt{2k}}{N}. \quad (31)$$

Umlauf and Burchard (2005) show that the limiting factor $c_{\text{min}}$ is a function of the steady-state Richardson number:

$$c_{\text{lim}} = \frac{(c_{\mu}^0)^3}{\sqrt{2}} \sqrt{\alpha_N(R_{st})} \quad (32)$$

The length scale limitation can be formulated as a limit on $\Psi$ (Warner et al., 2005)

$$\psi^{1/n} \leq \sqrt{2}c_{\text{lim}}(c_{\mu}^0)^{p/n} k^{m/n+1/2} N^{-1}. \quad (33)$$

Note that for negative $n$, (33) imposes a lower limit on $\psi$. In this work we limit $\Psi$ only, i.e. no limit is applied on $l$ or $\varepsilon$.

2.4. Stability functions

All the non-equilibrium stability functions are defined by a set of canonical parameters (Table 1 in Umlauf and Burchard, 2005). The functions can, however, be expressed as rational functions of $\alpha_M$ and $\alpha_N$ with parameters $n_i, d_i, n_{bi}$ (Umlauf and Burchard, 2005),

$$c_{\mu} = \frac{n_0 + n_1 \alpha_N + n_2 \alpha_M}{d_0 + d_1 \alpha_N + d_2 \alpha_M + d_3 \alpha_N \alpha_M + d_4 \alpha_N^2 + d_5 \alpha_M^2} \quad (34)$$

$$c_{\mu}' = \frac{n_{b0} + n_{b1} \alpha_N + n_{b2} \alpha_M}{d_0 + d_1 \alpha_N + d_2 \alpha_M + d_3 \alpha_N \alpha_M + d_4 \alpha_N^2 + d_5 \alpha_M^2} \quad (35)$$

Canuto et al. (2001) introduced two sets of full non-equilibrium stability functions, usually referred to as Canuto A and B. The stability region of Canuto B functions is somewhat larger than that of version A, suggesting that it is more robust in practice (Umlauf and Burchard, 2005). Another stability function, based on a very similar formulation, is given by Cheng et al. (2002).
2.4.1. Limiting $\alpha_M$ and $\alpha_N$

The stability functions are only defined for certain values of $\alpha_N$ and $\alpha_M$ due to numerical and physical reasons. First, the shear frequency $\alpha_M$ is positive by definition. To ensure its positivity $\alpha_N$ must be limited from below. The condition $\alpha_M = 0$ corresponds to the equilibrium relation $B = \varepsilon$, for which it holds (eq. A.23 in Umlauf and Burchard, 2005)

$$\frac{B}{\varepsilon} = -c'_\mu(\alpha_N)\alpha_N = 1. \quad (36)$$

This equilibrium condition corresponds to unstably stratified, convective regime where $\alpha_N < 0$ and $B > 0$. Substituting the stability function $c'_\mu$ into (36) results in

$$\alpha_{N_{\text{min}}} = \frac{-(d_1 + n_0) + \sqrt{(d_1 + n_0)^2 - 4d_0(d_4 + n_1)}}{2(d_4 + n_1)}. \quad (37)$$

Typical value of $\alpha_{N_{\text{min}}}$ is around -3.

Cropping $\alpha_N$ at the minimum value may lead to numerical oscillations as the gradient of the stability function is large for negative $\alpha_N$. Therefore a smoother transition has been proposed (eq. (19) in Burchard et al., 1999):

$$\tilde{\alpha}_N = \alpha_N - \frac{(\alpha_N - \alpha_c)^2}{\alpha_N + \alpha_{N_{\text{min}}} - 2\alpha_c}, \quad \forall \alpha_N < \alpha_c \quad (38)$$

The smoothness of the transition is controlled by $\alpha_c$, defined in range $\alpha_{N_{\text{min}}} < \alpha_c < 0$. Here a value $\alpha_c = -1.2$ is used.

In addition, the shear frequency, $\alpha_M$, must be limited above to ensure physically sound behavior and numerical stability (eq. 44 in Umlauf and Burchard, 2005; Burchard and Deleersnijder, 2001):

$$\alpha_{M_{\text{max}}} \approx \frac{d_0n_0 + (d_0n_1 + d_1n_0)\alpha_N + (d_1n_1 + d_4n_0)\alpha_N^2 + d_4n_1\alpha_N^3}{d_2n_0 + (d_2n_1 + d_3n_0)\alpha_N + d_3n_1\alpha_N^2} \quad (39)$$

Note that $\alpha_{M_{\text{max}}}$ depends on $\alpha_N$. In this work we first set $\alpha_N$ to $\tilde{\alpha}_N$ according to (38), and then apply the $\alpha_{M_{\text{max}}}$ limit.

2.5. Choosing empirical parameters

2.5.1. Computing $c_3^-$

The parameter $c_3^-$ controls the buoyancy production of $\Psi$ under stable stratification. Its value can be computed from (29):

$$c_3^- = c_2 - (c_2 - c_1) \frac{c'_\mu(R_{i_{\text{st}}}^t)}{c'_\mu(R_{i_{\text{st}}}^t)} \frac{1}{R_{i_{\text{st}}}^t} \quad (40)$$
To evaluate (40) one first needs to evaluate the stability functions under steady state. Using (30) one obtains a non-linear equation

$$c_\mu(\alpha_M, R_{st}^i)\alpha_M - c'_\mu(\alpha_M, R_{st}^i)\alpha_M R_{st}^i = 1 \quad (41)$$

from which $\alpha_M$ can be solved either analytically or numerically.

2.5.2. Parameters $c_\mu^0$ and $\sigma_\Psi$

Parameter $c_\mu^0$ stands for the value of the stability function in unstratified equilibrium where $P = \varepsilon$. Its value can therefore be computed for each stability function (eq. A.22 in Umlauf and Burchard, 2005).

In addition, a relation for the Schmidt number, $\sigma_\Psi$, and the von Karman constant $\kappa$ can be derived for the logarithmic boundary layer assumption (eq. 14 in Umlauf and Burchard, 2003):

$$\sigma_\Psi = \frac{n^2 \kappa^2}{(c_\mu^0)^2(c_2 - c_1)} \quad (42)$$

In this work we compute $\sigma_\Psi$ for each closure with $\kappa = 0.4$.

2.5.3. Setting minimum values for $k$ and $\varepsilon$

It is common to crop turbulent quantities to a small positive minimum value (Umlauf et al., 2005; Warner et al., 2005). The minimum values for $k$ and $\Psi$ are listed in Table 1. In addition we impose $l_{min} = 1.0 \times 10^{-12}$ m and $\nu_{min} = \nu'_{min} = 1.0 \times 10^{-8}$ m² s⁻¹. These limits are imposed after every update.

2.6. Positivity preserving time discretization

The prognostic variables $k$ and $\Psi$ are non-negative by definition. The discretized system must maintain the non-negativity of these variables at all times to ensure physically sound and numerically stable solution. To this end, the production-destruction terms in equations (1) and (2) require special treatment.

For convenience we re-write the governing equations in the form

$$\frac{\partial k}{\partial t} + A_k(k, u, w) = D_k(k, \nu) + S_k(k, \varepsilon, \nu, \nu', M, N) \quad (43)$$

$$\frac{\partial \Psi}{\partial t} + A_\Psi(\Psi, u, w) = D_\Psi(k, \nu) + S_\Psi(\Psi, \varepsilon, \nu, \nu', M, N) \quad (44)$$
Table 1: List of parameter values for three different turbulence closure models. $k – \varepsilon$ and $k – \omega$ values (indicated by †) are from Tables 1 and 2 in Umlauf and Burchard (2003); The gen model values (indicated by *) corresponds to the first line in Table 7 in Umlauf and Burchard (2003). In all cases, $c_3^-$ and $c_{lim}$ are computed numerically from (40) and (32), respectively; $\sigma_\psi$ and $c_0^\mu$ are computed as detailed in Section 2.5.2. The shown values correspond to the Canuto A stability functions.

| Parameter | $k – \varepsilon$ | $k – \omega$ | gen |
|-----------|-------------------|---------------|-----|
| $p$       | 3†                | -1.0†         | 2.0*|
| $m$       | 1.5†              | 0.5†          | 1.0*|
| $n$       | -1.0†             | -1.0†         | -0.67*|
| $\sigma_k$ | 1.0†             | 2.0†          | 0.8*|
| $\sigma_\psi$ | 1.20†             | 2.072†        | 1.18*|
| $c_1$     | 1.44†             | 0.555†        | 1.0*|
| $c_2$     | 1.92†             | 0.833†        | 1.22*|
| $c_3^+$   | 1.0               | 1.0           | 1.0 |
| $c_3^-$   | -0.629            | -0.643        | 0.052|
| $R_i^{st}$ | 0.25              | 0.25          | 0.25|
| $c_0^\mu$ | 0.5270            | 0.5270        | 0.5270|
| $\kappa$  | 0.4               | 0.4           | 0.4 |
| $c_{lim}$ | 0.267             | 0.267         | 0.267|
| $k_{min}$ | 1.0×10^{-6}       | 7.6×10^{-6}   | 1.0×10^{-6}|
| $\psi_{min}$ | 1.0×10^{-14}   | 1.0×10^{-14} | 1.0×10^{-14}|

where $A_i$, $i = \{k, \Psi\}$, denote the horizontal and vertical advection terms, $D_i$ the vertical diffusion terms, and $S_i$ the source terms:

$$S_k = P + B - \varepsilon$$  \hspace{1cm} (45)

$$S_\Psi = \frac{\Psi}{k} (c_1 P + c_3 B - c_2 \varepsilon).$$  \hspace{1cm} (46)

Positivity preserving schemes are based on the Patankar treatment where all sink terms (i.e., $S < 0$) are treated implicitly (Patankar, 1980; Burchard et al., 2003). In the $k$ equation, the shear production term, $P$, and TKE dissipation rate, $\varepsilon$, are always positive, resulting in a source and sink term,
respectively. The sign of the buoyancy production term, \( B \), on the other hand, depends on the sign of \( N^2 \). We therefore split the term in two parts: \( B = B_+ + B_- \) with \( B_+ \geq 0 \) and \( B_- < 0 \):

\[
B_+ = -\nu'N^2, \quad \forall N^2 < 0 \quad (47) \\
B_- = -\nu'N^2, \quad \forall N^2 \geq 0 \quad (48)
\]

In the \( \Psi \) equation we have \( c_1 P \geq 0 \) and \( c_2 \varepsilon \geq 0 \). In this case the sign of the \( B \) term, however, also depends on the parameter \( c_3^+ \): \( c_3^+ \) is used when \( B \geq 0 \), and \( c_3^- \) when \( B < 0 \). Noting that \( c_3^+ > 0 \), we can split the source terms as follows:

Case \( c_3^- \geq 0 \) :
\[
(c_3 B)_+ = c_3^+ B_+ \quad (49) \\
(c_3 B)_- = c_3^- B_- \quad (50)
\]

Case \( c_3^- < 0 \) :
\[
(c_3 B)_+ = c_3^+ B_+ + c_3^- B_- \quad (51) \\
(c_3 B)_- = 0 \quad (52)
\]

Considering a single state, first order time discretization, we can write the positivity preserving time discretization as

\[
\frac{k^{n+1} - k^n}{\Delta t} + A_k^n - D_k^{n+1} = P^n + B^n_+ + \frac{k^{n+1}}{k^n} (B^n_- - \varepsilon^n) \quad (S_n^+)^n + (S_n^-)^{n+1} \quad (53)
\]

\[
\frac{\Psi^{n+1} - \Psi^n}{\Delta t} + A_{\Psi}^n - D_{\Psi}^{n+1} = \psi^n + (c_1 P^n + (c_3 B)^n_+) + \frac{\Psi^{n+1}}{k^n} ((c_3 B)^n_- - c_2 \varepsilon^n) \quad (S_{\Psi}^+)^n + (S_{\Psi}^-)^{n+1} \quad (54)
\]

The equations are linear with respect to the solution \( k^{n+1} \) and \( \Psi^{n+1} \). Note that in (53) we have employed the Patankar treatment, i.e. scaled the sink term \( S_k^- \) with the ratio \( k^{n+1} / k^n \) to render it implicit.

3. Finite element discretization

3.1. Thetis coastal ocean model

The turbulence closure model was implemented in the Thetis three-dimensional circulation model [Kärnä et al. 2018]. Thetis solves the hydrostatic equations with a semi-implicit DG finite element method. The equations are
solved in a time-dependent 3D mesh, unstructured in the horizontal direction. A second-order split-implicit time integration scheme is used to advance the equations in time; the mesh movement is implement with the Arbitrary Lagrangian–Eulerian (ALE) method. Horizontal advection of 3D fields is solved with a Strong Stability-Preserving SSPRK(2,2) scheme (Shu and Osher, 1988). Vertical diffusion is treated implicitly. The model formulation is described in detail in Kärnä et al. (2018).

Turbulent quantities are advanced in time similarly to other 3D fields: Horizontal advection is solved with the same SSPRK(2,2) scheme that is used for tracers and 3D velocity. Vertical dynamics of $k$ and $Ψ$ are solved implicitly. As the vertical problem is generally stiff, it is crucial to use an L-stable implicit method to avoid spurious oscillations (Hairer and Wanner, 1996). It is worth noting that the commonly-used Crank-Nicolson scheme is not L-stable and may lead to unphysical solutions. The simplest choice is the first order Backward Euler method (used in Kärnä et al. (2018) for example). This scheme is, however, known to be dissipative. In this work a two-stage, second-order diagonally implicit Runge-Kutta scheme, DIRK(2,3,2) (Ascher et al., 1995), is used. The DIRK scheme involves two implicit solves per time step and is thus roughly twice as expensive compared to the Backward Euler scheme. The same DIRK scheme is used for the vertical diffusion of tracers and 3D velocity as well.

Thetis source code is freely available. We have also archived the exact source code version used to to produce the results in this paper (see Appendix A).

3.2. Mathematical notation

Let $Ω$ be the three-dimensional domain that spans from the sea floor $z = -h(x, y)$ to the free surface $z = η(x, y)$; the bottom and top surfaces are denoted by $Γ_b$ and $Γ_s$, respectively.

The domain $Ω$ is divided into three-dimensional elements $e ∈ P$. The mesh is generated by extruding a two-dimensional surface mesh over the vertical dimension. The surface mesh consist of either triangles or quads, resulting in triangular prisms, or hexahedron 3D elements, respectively.

The set of horizontal and vertical interfaces are denoted by $I_h$ and $I_v$, respectively. The outward unit normal vector is denoted by $n = (n_x, n_y, n_z)$; its restriction on the horizontal and vertical interfaces are denoted by $n_h$, and $n_v$, respectively. The vertical facets $I_v$ are strictly vertical, implying $n_v = (n_x, n_y, 0)$. 
In the weak forms we use the following notation for volume and interface integrals

\[
\langle \bullet \rangle_\Omega = \int_\Omega \bullet \, dx, \tag{55}
\]

\[
\llangle \bullet \rrangle_{\partial \Omega} = \int_{\partial \Omega} \bullet \, ds. \tag{56}
\]

In interface terms we additionally use the average \{ \cdot \} and jump \[ \cdot \] operators for scalar \( a \) and vector \( u \) fields:

\[
\llangle a \rrangle = \frac{1}{2}(a^+ + a^-), \tag{57}
\]

\[
[u] = \frac{1}{2}(u^+ + u^-), \tag{58}
\]

\[
[a n] = a^+ n^+ + a^- n^-, \tag{59}
\]

\[
[u \cdot n] = u^+ \cdot n^+ + u^- \cdot n^-, \tag{60}
\]

\[
[un] = u^+ n^+ + u^- n^-, \tag{61}
\]

where the superscripts ‘+’ and ‘−’ arbitrarily label the values on either side of the interface.

### 3.3. Discontinuous Galerkin discretization of the GLS equations

The prognostic variables of the 3D system (1, 2) are \( k \) and \( \Psi \). Diagnostic variables include the dissipation rate \( \varepsilon \), turbulent length scale \( l \), vertical eddy viscosity \( \nu \), and diffusivity \( \nu' \). Diagnostic variables originating from the 3D circulation model are the vertical shear frequency \( M \) and buoyancy frequency \( N \). The choice of function spaces where these variables reside is crucial for numerical stability and accuracy.

In this work we use the degree zero discontinuous Galerkin elements for all the variables (see Table 2). That is, the variables belong to a function space \( W = P_{DG}^0 \times P_{DG}^0 \) (here the \( \times \) operator stands for the Cartesian product of function spaces in the extruded mesh: horizontal \( \times \) vertical function space).

Let \( \psi \in \mathcal{W} \) be a test function. The weak formulations are derived by taking the continuous equations (1-2), multiplying them by \( \psi \), and integrating over the domain \( \Omega \). The weak formulation then reads: find \( k, \Psi \in \mathcal{W} \) such that
Table 2: Prognostic and diagnostic variables and their function spaces. The shear and buoyancy frequencies, $M$ and $N$, are computed diagnostically from the state variables of the hydrodynamical model, and fed to the GLS model as inputs. Viscosity and diffusivity, $\nu$ and $\nu'$, on the other hand, are fed to the hydrodynamical model.

**GLS Model**

| Prognostic variables | Field | Symbol | Equation | Function space |
|----------------------|-------|--------|----------|----------------|
| Turbulent kinetic energy | $k$ | (1) | $P_{DG}^0 \times P_{DG}^0$ |
| Length scale | $\Psi$ | (2) | $P_{DG}^0 \times P_{DG}^0$ |
| Diagnostic variables | TKE dissipation rate | $\varepsilon$ | (8) | $P_{DG}^0 \times P_{DG}^0$ |
| Turbulent length scale | $l$ | (9) | $P_{DG}^0 \times P_{DG}^0$ |
| Eddy viscosity | $\nu$ | (10) | $P_{DG}^0 \times P_{DG}^0$ |
| Eddy diffusivity | $\nu'$ | (11) | $P_{DG}^0 \times P_{DG}^0$ |

**Hydrodynamical model**

| Prognostic variables | Field | Symbol | Equation | Function space |
|----------------------|-------|--------|----------|----------------|
| Horizontal velocity | $\mathbf{u}$ | (24-25) in TK2018 | $[P_{DG}^1 \times P_{DG}^1]^2$ |
| Temperature | $T$ | (26) in TK2018 | $P_{DG}^1 \times P_{DG}^1$ |
| Salinity | $S$ | (26) in TK2018 | $P_{DG}^1 \times P_{DG}^1$ |
| Diagnostic variables | Density | $\rho$ | (14) in TK2018 | $P_{DG}^1 \times P_{DG}^1$ |
| Shear frequency | $M$ | (5) | $P_{DG}^0 \times P_{DG}^0$ |
| Buoyancy frequency | $N$ | (6) | $P_{DG}^0 \times P_{DG}^0$ |

$$
\frac{\partial}{\partial t} \left( k\psi \right)_{\Omega} + A_{h,k} + A_{v,k} = D_k + S_k, \ \forall \psi \in \mathcal{W}, \quad (62)
$$

$$
\frac{\partial}{\partial t} \left( \Psi\psi \right)_{\Omega} + A_{h,\Psi} + A_{v,\Psi} = D_\Psi + S_\Psi, \ \forall \psi \in \mathcal{W}, \quad (63)
$$

where $A_{h,i}$ and $A_{v,i}$, $i = k, \Psi$ denote the horizontal and vertical advection terms, while $D_i$ and $S_i$ are the diffusion and source terms, respectively.
The advection terms are discretized with standard DG upwind technique as implemented in the hydrodynamical model (Karä et al., 2018). The diffusion terms are treated with Symmetric Interior Penalty Galerkin method (SIPG; Epshteyn and Rivièere, 2007) with a penalty factor $\sigma = 1/L$ where $L$ is the vertical element size (Karä et al., 2018).

The source terms are split to sources and sinks using equations (53-54):

$$S_k = \left< S_k^+ \psi \right>_{\Omega} + \left< S_k^- \psi \right>_{\Omega}$$  \hspace{1cm} (64)

$$S_\psi = \left< S_\psi^+ \psi \right>_{\Omega} + \left< S_\psi^- \psi \right>_{\Omega}$$  \hspace{1cm} (65)

Let $\psi_i$ be the basis of the function space $W$. We require that the solution belongs to this space, i.e. $k, \Psi \in W$, and use the finite element approximations (e.g., $k = \sum_i k_i \psi_i$). Using the basis functions as test functions, we can write (62-63) in a bilinear form:

$$\frac{\partial}{\partial t} (\operatorname{M}k) + A_{h,k} + A_{v,k} = D_k + S_{+,k} + S_{-,k}, \quad \forall \psi_j \in W$$  \hspace{1cm} (66)

$$\frac{\partial}{\partial t} (\operatorname{M}\Psi) + A_{h,\Psi} + A_{v,\Psi} = D_\Psi + S_{+,\Psi} + S_{-,\Psi}, \quad \forall \psi_j \in W$$  \hspace{1cm} (67)

where $[\operatorname{M}]_{i,j} = \left< \psi_i \psi_j \right>_{\Omega}$ is the mass matrix, and the other terms are also bilinear, e.g, $D_k = D_k(\psi_i, \psi_j)$.

### 3.4. Computing shear and buoyancy frequencies

Computing the vertical shear and buoyancy frequencies accurately is crucial for maintaining numerical stability (Karä et al., 2012). We compute the vertical gradients weakly. Denoting the shear frequency vector by $\operatorname{M} = \frac{\partial \mathbf{u}}{\partial z}$ we define

$$\left< \operatorname{M} \cdot \psi \right>_{\Omega} = \left< \mathbf{u} \cdot \frac{\partial \psi}{\partial z} \right>_{\Omega} + \left< \{ \mathbf{u} \} \cdot [\psi_n] \right>_{\Gamma_h} + \left< \mathbf{u} \cdot \psi_n \right>_{\Gamma_s \cup \Gamma_b}$$  \hspace{1cm} (68)

$$M^2 = |\operatorname{M}|^2,$$  \hspace{1cm} (69)
Analogously, we can compute the \( \frac{\partial \rho'}{\partial z} = R_z \)

\[
\langle R_z \psi \rangle_{\Omega} = -\langle \rho' \frac{\partial \psi}{\partial z} \rangle_{\Omega} + \langle \langle \rho' \rangle \psi n_z \rangle_{\Gamma_b} + \langle \langle \rho' \psi n_z \rangle \rangle_{\Gamma_s \cup \Gamma_b}
\]
\[
N^2 = -\frac{g}{\rho_0} R_z.
\]

3.5. Time integration

For convenience we re-write the \( k \) and \( \Psi \) weak forms as

\[
\frac{\partial k}{\partial t} = F_k(k, u, w) + G_k(k, \varepsilon, \nu, \nu', M, N) \tag{72}
\]
\[
\frac{\partial \Psi}{\partial t} = F_\Psi(\Psi, u, w) + G_\Psi(\Psi, k, \varepsilon, \nu, \nu', M, N) \tag{73}
\]

where \( F_k \) and \( F_\Psi \) contain the advection terms whilst \( G_k \) and \( G_\Psi \) contain the vertical diffusion and source terms.

The solution can then be split in explicit advection stage and implicit vertical dynamics stage. The explicit stage is solved with SSPRK(2,2) scheme (Kärnä et al., 2018):

\[
k^{(1)} = k^n + \Delta t \tilde{F}_k(k^n, u^n, w^n - w_{m}^{(1)}),
\]
\[
\tilde{k}^{n+1} = k^n + \Delta t \left( \frac{1}{2} \left( \tilde{F}_k(k^n, u^n, w^n - w_{m}^{(1)}) + \tilde{F}_k(k^{(1)}, u^{(1)}, w^{(1)} - w_{m}^{n+1}) \right) \right).
\]

where \( w_m \) denotes the vertical mesh velocity and \( \tilde{F} \) denotes the ALE weak forms of \( F_k \) terms (see Kärnä et al. (2018)). The advection stage for \( \Psi \) is derived analogously.

The implicit stage reads:

\[
k^{n+1} = \tilde{k}^n + \Delta t \tilde{G}_k(k^{n+1}, \varepsilon^n, \nu^n, \nu'^n, M^n, N^n),
\]
\[
\tilde{\Psi}^{n+1} = \tilde{\Psi}^n + \Delta t \tilde{G}_\Psi(\Psi^{n+1}, k^n, \varepsilon^n, \nu^n, \nu'^n, M^n, N^n).
\]

This system is solved with the two-stage DIRK(2,3,2) method. The full time integration scheme is summarized in Algorithm 1.
Algorithm 1 Summary of the coupled time integration algorithm.

**Require:** Model state variables at time $t_n$: $\eta, \bar{u}, T, S, u', k, \Psi$

**First stage:**
1. Solve 2D system: $\eta^{(1)}, \bar{u}^{(1)}$
2. Solve explicit 3D ALE problem: $T^{(1)}, S^{(1)}, u'^{(1)}, k^{(1)}, \Psi^{(1)}$
3. Update 2D coupling term, density, and vertical velocity

**Second stage:**
4. Solve 2D system: $\eta^{n+1}, \bar{u}^{n+1}$
5. Solve explicit 3D ALE problem: $\tilde{T}^{n+1}, \tilde{S}^{n+1}, \tilde{u}^{m+1}, \tilde{k}^{n+1}, \tilde{\Psi}^{n+1}$
6. Update 2D coupling term

**Final stage:**
7. Solve mean flow vertical dynamics implicitly: $T^{n+1}, S^{n+1}, u'^{n+1}$
8. Update density, vertical velocity, bottom friction
9. Solve turbulence vertical dynamics implicitly: $\Psi^{n+1}, k^{n+1}$
10. Update diagnostic turbulence fields: $l^{n+1}, \varepsilon^{n+1}, \nu^{n+1}, \nu'^{n+1}$

4. Results

We verify the GLS implementation with a series of standard turbulence closure test cases. All the test have been carried out with the $k - \varepsilon$, $k - \omega$, and the gen models as described in Table 1.

4.1. Bottom friction

The first test is an open channel with bottom friction. The fluid is initially at rest, forced only by a constant free surface slope $\partial \eta/\partial x = -1 \times 10^{-5}$. In the absence of rotation, the flow converges to a steady state solution where the pressure gradient is balanced by the bottom friction.

Near the bed the flow velocity follows the well-known logarithmic profile, which can be expressed as (e.g. [Hanert et al., 2007])

$$u(z) = \frac{u_b^*}{\kappa} \log \left( \frac{z^b + z + h}{z^b_0} \right)$$  \hspace{1cm} (78)

where $u_b^*$ is the bottom friction velocity and $z^b_0 = 1.5 \times 10^{-3}$ m is the bottom roughness. The bottom friction velocity can be solved from the momentum balance:
\[ u_b^* = \sqrt{gH \left| \frac{\partial \eta}{\partial x} \right|}. \] (79)

The eddy viscosity follows a parabolic profile

\[ \nu = -\frac{u_b^*}{H} \kappa (z^b_0 + z + h) z \] (80)

At the bed the conventional quadratic friction law is imposed

\[ \nu \frac{\partial u}{\partial z} = C_d \| \mathbf{u}_b \| \mathbf{u}_b, \] (81)

\[ C_d = \frac{\kappa^2}{\log(z^b_0 + z + h)^2} \] (82)

where \( C_d \) is the drag coefficient, \( z_b \) is the \( z \)-coordinate at the middle of the bottom most element, and \( \mathbf{u}_b = \mathbf{u}(z_b) \).

The free flow was simulated in a 5.0 km wide square domain with constant 15 m depth. Horizontal mesh resolution was 2.5 km. Periodic boundary conditions were used in the \( x \) direction. Initially the flow is at rest. A steady state solution is reached after roughly 12 h of simulation. All simulations were carried out with 25 s time step.

First, we experimented the three closure models, GLS, \( k - \varepsilon \), and \( k - \omega \) with Canuto A stability functions. Vertical profiles of velocity, TKE, \( \varepsilon \), \( l \), and viscosity are shown in Figure 1. In all simulations 250 vertical levels were used. The velocity profile is close to the analytical logarithmic solution in all cases. TKE shows the expected nearly linear profile. In terms of eddy viscosity, the \( k - \omega \) model matches best to the analytical solution. GLS and \( k - \varepsilon \) models tend to overestimate viscosity in the upper water column, while underestimating it in the middle. This behavior is in-line with other results in the literature (Warner et al., 2005). One possible cause for this deviation is the surface boundary condition for \( \Psi \), which affects both \( \Psi \) and \( l \) near the free surface (Figure 1d).

Second, the \( k - \omega \) model was run with different vertical grids consisting of 5, 25, and 250 levels (Figure 2). The velocity profiles are close to the analytical solution for all the resolutions. As resolution is increased viscosity
converges to a parabola close to the analytical solution. This test demonstrates that the effective friction felt by the water column does not depend strongly on the vertical resolution. In addition, it shows that the numerical solver remains stable even with small vertical elements (6 cm).

Third, we experimented with the different stability functions. We ran the $k - \omega$ model with Canuto A, B and Cheng stability functions (Figure 3). In general the choice of the stability function does not have a major impact on the results. The results of Canuto A and Cheng stability functions are nearly identical. Canuto B functions, on the other hand, yielded slightly larger viscosity, and consequently lower velocity. The effect of stability functions was similar with other closure models as well (not shown).

4.2. Wind-driven entrainment

The next test examines mixed layer deepening due to surface stress, based on the laboratory experiment originally conducted by Kato and Phillips (1969). Initially the water column is at rest and linearly stratified. A constant surface stress is applied at the free surface. Stress induced mixing leads into a homogeneous surface layer that grows deeper in time. The depth of the mixed layer follows the empirical formula suggested by Price (1979):

$$h = \frac{1}{2} \left( \frac{u}{\tau_b} \right)^{-2}$$

where $h$ is the depth of the mixed layer, $u$ is the surface stress, and $\tau_b$ is the friction stress.
Figure 2: Bottom friction test with varying number of levels. The $k-\omega$ closure with Canuto A stability functions was used. Black dashed line stands for the analytical velocity and viscosity profiles.

\[ d_{\text{ML}} = 1.05 \ u_s^* \sqrt{\frac{t}{N_0}} \quad (83) \]

where $u_s^*$ is the surface friction velocity and $N_0$ is the initial spatially invariable buoyancy frequency. Here values $u_s^* = 0.01 \text{ m s}^{-1}$ and $N_0 = 0.01 \text{ s}^{-1}$ are used. $N_0$ is prescribed by imposing a suitable linear salinity field and using a linear equation of state.

The mixed layer deepening was simulated in 5 km wide square domain with constant 50 m depth and 2.5 km mesh resolution. All simulations were carried out with 30 s time step.

First three different mesh resolutions, $\Delta z = 0.2, 0.5, \text{ and } 1.0 \text{ m}$, were experimented with, resulting in 250, 100, and 50 vertical levels, respectively. The evolution of the mixed layer depth is presented in Figure 4 for $k-\varepsilon$ model and Canuto A stability functions. All resolutions result in mixed layer deepening that is in good agreement with the empirical formula (83).
Figure 3: Bottom friction test with different stability functions. In all cases the $k - \omega$ closure were used. Canuto A and Cheng functions yield nearly identical results. Black dashed line stands for the analytical velocity and viscosity profiles.

Next we tested the three different turbulence closure models (with Canuto A stability functions) on the medium resolution $\Delta z = 0.5$ m mesh (Figure 5). All models reproduce a realistic mixed layer depth. The $k - \varepsilon$ and GLS models are close to the empirical mixed layer depth. The $k - \omega$ model tends to under estimate the mixed layer depth, especially in the beginning of the simulation, but the difference is small. These results are in good agreement with previous studies (e.g. Warner et al. 2005, Kärnä et al. 2012).

We also carried out experiments with different stability functions (not shown); in all cases, the mixed layer depth behaved correctly, its variance being similar to what is seen in Figure 5.

4.3. Idealised estuary

Estuarine circulation is an essential feature in coastal domains. It is dominated by the interplay of buoyancy driven stratification and vertical mixing. Buoyancy input from a river tends to tilt isopycnals and increase stratification in the estuary. On the other hand, bottom stress induced vertical

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mixing tends to decrease stratification and mix the water column. Under sufficiently strong stratification, turbulence cannot penetrate the pycnocline resulting in a well mixed bottom layer that is de-coupled from the surface layer. The competition between these two tendencies cannot be modeled without a two-equation turbulence closure model.

We test the model’s capability of representing estuarine circulation with the idealized estuary test case by Warner et al. (2005). This test case has been used to validate other models as well, e.g. SLIM (Kärnä et al. 2012), and SELFE (Lopez and Baptista 2017).

The domain is a rectangular channel 100 km long and 1 km wide. Depth varies linearly from 10 m at the deep (ocean) boundary to 5 m in the shallow (river) end. Horizontal mesh resolution is 500 m; 20 equally distributed vertical levels are used.

At the river boundary a constant discharge of \( F_{\text{river}} = 400 \text{ m}^3 \text{ s}^{-1} \) is imposed, corresponding to a 8 cm s\(^{-1} \) seaward velocity. Water elevation is unprescribed, and water salinity is set to zero. At the ocean boundary
Figure 5: Mixed layer depth in wind-driven entrainment test with different turbulence closures. The blue, yellow, and green line stand for $k - \varepsilon$, $k - \omega$, and GLS models, respectively. In all cases the Canuto A stability functions were used. The mixed layer depth was defined as the highest point where $k > 10^{-5} \text{ m}^2 \text{ s}^{-2}$. In all cases the Canuto A stability functions were used. Black dashed line stands for the empirical formula \[83].

A sinusoidal tidal current is imposed with 0.4 m s$^{-1}$ amplitude and period $T_{\text{tide}} = 12$ h. In addition, the seaward volume flux $F_{\text{river}}$ is applied at ocean boundary to ensure tidally averaged volume conservation. Salinity of inflowing ocean water is set to is 30 psu. Throughout the simulation temperature is kept at constant 10 °C.

Initially water is at rest. Salinity varies from 30 to 0 psu along the channel between 30 and 80 km from the ocean boundary (Figure 6 (a)). The ocean and river boundary conditions are ramped up for one hour. During the simulation estuarine circulation quickly develops, driving freshwater seaward in the surface layer. A thick salt wedge forms, oscillating with the tides. The model is spun up for 15 days after which the solution has reached a quasi-periodic state where each tidal cycle is nearly identical.

Figure 6 shows the instantaneous salinity distribution after 16 days of simulation for $k - \varepsilon$ (b), $k - \omega$ (c) and GLS models (d). In all simulations the Canuto A stability functions were used. The results show a thick salt wedge, and a fairly thin, seaward flowing surface layer. Salinity reaches about 80 km from the estuary mouth. The $k - \omega$ model shows lower stratification
Figure 6: Idealized estuary simulation. a) Initial condition for salinity. b) Salinity field after 16 days of simulation for the $k - \varepsilon$ (b), $k - \omega$ (c), and GLS model (d). Canuto A stability functions were used in all simulations.

and shorter salinity intrusion indicating stronger effective mixing. The GLS model results in the shortest salinity intrusion.

Vertical profiles are presented in Figure 7 for the three closures. The profiles indicate that the well-mixed bottom layer fills most of the water column. In the upper water column stratification is very strong which limits mixing and results in almost turbulence-free surface layer. Salinity profiles
in Figure 7 (a) show that stratification is indeed weaker in the $k-\omega$ model. It also generates higher TKE and viscosity in the bottom layer suggesting a larger overall (tidally-averaged) mixing. The $k-\varepsilon$ and GLS model behave quite similarly. GLS, however, generates lower TKE and viscosity which is consistent with the shorter salinity intrusion (Figure 6).

Qualitatively the presented results are similar to those in Warner et al. (2005), Kärnä et al. (2012) and Lopez and Baptista (2017). Some differences do exist in salinity intrusion and stratification, for example, as the flow is very sensitive to the ocean boundary conditions and, more generally, the model’s discretization. It should also be noted that the behavior of the three turbulence closure models strongly depends on the chosen parameters.

4.4. Application to Columbia River plume

The Columbia River is a major freshwater source in the west coast of the United States (Figure 8). With annual mean discharge of 5500 m$^3$ s$^{-1}$ it is the second largest river in continental USA (Chawla et al., 2008). Maximal daily tidal range varies between from less than 2.0 to 3.6 m at the river mouth (Kärnä et al., 2015). The river plume is a major feature in the Pacific Northwest Coast, affecting stratification, currents, and nutrients in the coastal waters (Hickey and Banas, 2003).

The river plume can be divided into different water masses. Horner-Devine et al. (2009) define four water masses: the source water, followed by the tidal, re-circulating, and far-field plume. The tidal plume (with 6 to 12 h
time scale) consists of a freshwater lens being emitted from the river mouth every tidal cycle. Once released, it rapidly spreads out and becomes thinner, its depth ranging from 6 to 3 m. Salinity is below 21 psu. The tidal plume eventually merges with the re-circulating plume.

The re-circulating plume forms an anticyclonic bulge at the vicinity of the river mouth. In the cross-shore direction, the bulge is roughly 40 km in diameter. The re-circulating plume consists of freshwater volume equivalent to 3–4 days of river discharge; salinity is between 21 and 24 psu.

The far-field plume lies beyond the re-circulating plume. It is the zone where final mixing of the plume and ambient ocean waters takes place, unaffected by the momentum of the river discharge. Typically, the far-field plume forms a large coastal current, driven by buoyancy and Earth’s rotation, that can extend hundreds of kilometers North from the river mouth. The evolution of the far-field plume, however, is strongly affected by winds and coastal currents.

The typical northward propagation of the river plume can be arrested
by northerly, upwelling-favorable winds. Upwelling generates an off-shore current in the surface layer, eroding the river plume from the coast. The plume detaches from the coast, spreads out and becomes thinner. Under sufficiently strong and prevailing winds, the plume begins to travel southwest. Northerly winds are more common in the Pacific Northwest during summer months, which is why the southwest-oriented plume is often called the summer plume. Upwelling-favorable winds, therefore, can reverse the orientation of the plume.

Southerly, downwelling-favorable winds, on the other hand, enhance the northward coastal current. Under downwelling conditions, the surface layer flows onshore and pushes the plume against the coast, making it narrower and thicker. Consequently, the coastal current becomes more pronounced: it becomes narrower and propagates faster towards the North.

The evolution of the river plume was simulated with Thetis. The computational domain spans from roughly 40°N to 50°N in the zonal direction (Figure 8). The western boundary is located roughly 100 km west of the coast. The Columbia River is included in the domain, excluding the shallow lateral bays. The river boundary is located at Beaver Army, 86 km upstream from the mouth. The horizontal mesh resolution (triangle edge length) ranges from roughly 900 m in the estuary to 15 km at the open ocean boundaries. In the vertical direction, 20 terrain-following layers were used. The layer thickness ranges from roughly 1 m near the surface to a maximum of 180 m at the bottom. The entire vertical grid adjusts to the free surface similarly to $z^*$ grid used in structured grid models (Adcroft and Campin, 2004).

We used a composite bathymetry data (Kärnä and Baptista, 2016a) that was interpolated on the model grid (Figure 8). In addition, the bathymetry was smoothed with a Laplacian diffusion operator to limit strong gradients which could introduce internal pressure errors. Minimum water depth was set to 3.5 m. Wetting and drying was neglected.

Atmospheric pressure and 10 m wind were obtained from the North American Mesoscale Model (NAM) model. Wind stress was computed with the formulation by Large and Pond (1981). At the ocean boundary temperature, salinity and sub-tidal velocity was imposed from the global Navy Coastal Ocean Model (NCOM) model (Barron et al. 2006). In addition, tidal elevation and velocities were imposed from the TPXO v9.1 model (Egbert and Erofeeva, 2002). At the river boundary discharge and water temperature are imposed using US Geological Survey (USGS) gauge data. Salinity is set to zero.
The simulation covers a time period from May 1 2006 to July 2. The first month is used to spin up the simulation; the analysis period is from June 1 onward. This spin-up time is sufficient for the estuary–plume system: The estuary has a residence time of a few days (Kärnä and Baptista, 2016b); As stated above, the far-field plume develops in a couple of weeks.

Thetis model was compared against a SELFE hindcast simulation (Kärnä and Baptista, 2016a). SELFE has been used to model the Columbia River system for over a decade. Its skill has been analyzed in the tidal river and estuary (Kärnä et al. 2015; Kärnä and Baptista, 2016a) as well as in the plume (Chawla et al. 2008). SELFE model uses a higher resolution mesh, element size being of the order 200 m in the estuary. The vertical grid consists of 37 terrain-following $S$ levels in the upper 100 m, and at most 17 $z$ levels below. Time step is 36 s. For more detailed information on the model configuration, see Kärnä and Baptista (2016a).

Figure 9: Time series of wind, tidal and river forcings in the Columbia River plume application. The northward wind component (a) is from the atmospheric model at the rice station; The tidal elevation (b) is from tpoin tide gauge; River discharge (c) is from Beaver Army gauge. The shaded areas indicate strong downwelling periods.

Figure 9 shows the atmospheric and fluvial forcing conditions for the analysis period. Winds alternate between up- (northerly) and downwelling-favorable direction (Figure 9a). Tides exhibit a typical spring-neap variation
to the system, tidal range varying between 1.6 and 3.4 m; River discharge is roughly 10000 m$^3$ s$^{-1}$ during the simulation (Figure 9 b and c).

Figure 10: Time series of observed surface salinity at selected stations in the Columbia River application. The shaded areas indicate strong upwelling periods. The station locations are shown in Figure 8.

Figure 10 shows time series of observed surface salinity at stations rino, rice, and ogi01. The rice station (Figure 10 b) is located in the tidal plume recording the passing of each tidal freshwater lens. Both Thetis and SELFE replicate the sub-tidal and tidal evolution variability of the near field plume very well. Note that exact replication of the tidal signal is difficult as salinity gradients are very large. Measured salinity therefore strongly depends on the passing of the plume fronts, which is sensitive to atmospheric forcing, mesh resolution, mixing, and bathymetry features, for instance.

The ogi01 station (Figure 10 c) is located some 25 km southeast from the river mouth. It captures the re-circulating plume when it is pushed southward from the river mouth; Typically this occurs during southerly winds. During the simulation period, two of such events are recorded, on June 6–10 and June 18–20. Both models can capture the southward transport of the plume relatively well.

The northern station, rino, is located in the far-field plume region, 24 km
off the coast (Figure 10 a). The narrow coastal current, however, is often situated closer to the coast. The plume passes through rino station only in cases where the winds erode the plume from the coast; Such events are seen in the observations on June 6 and 18. The Thetis simulation captures those events well, although the arrival of the plume is delayed by roughly one day. Salinity in Thetis also tends to be higher compared to the observations. Surface salinity in SELFE, on the other hand, varies very slowly and shows only small variation during the latter June 18 event. The lack of pronounced fronts in SELFE results suggests stronger mixing.

Figure 11 shows the evolution of the surface salinity in the Thetis simulation. Prior to the first event (panels a and b), the bulge of the re-circulating plume is clearly visible just north of the river mouth. The far-field plume is quite narrow and fresh; it travels northward by the coast and does not reach the rino station. On the onset of northerly winds (panels c and d), the far-field plume detaches from the coast, spreads out, and passes through the station. As the winds prevail, the plume spreads out more and starts to travel southwest (panels e - h). Eventually, a new coastal plume starts to develop. Note that in response to the winds, the re-circulating plume also spreads out, dilutes and begins to meander.

Surface salinity comparison against SELFE model is shown in Figure 12. The plume in SELFE model does respond to the winds in a similar fashion: it spreads out and begins to travel southwest (panels d - f). The plume, however, is very diffused compared to Thetis: While there are quite strong frontal features in the tidal plume region, they quickly dissipate. Overall the plume lacks fronts, eddies, and filaments, indicating much larger effective mixing. Due to the mixing, the coastal plume is too wide and it travels northward too slowly. The plume is also deeper and less stratified compared to Thetis (not shown).

5. Discussion

We have presented a coupled circulation-turbulence model based on DG finite element discretization. The idealized bottom friction and mixed layer deepening experiments show that the model captures both bottom boundary layer and mixed layer dynamics correctly. It can simulate entrainment processes under strong vertical shear and stratification conditions. No numerical artifacts arise even with very high vertical resolution. The idealized estuary test case verifies that the coupled circulation-turbulence model can repro-
duce realistic estuarine circulation, and remains stable in strongly stratified, rapidly changing flows. Overall the model’s performance is in good agreement with results presented in the literature (e.g. Warner et al. 2005; Kärnä et al. 2012).

All the tested closure models and stability functions yield similar results, although some differences do appear. For example, the differences in the bottom friction test case between different closures (Figure 1) are mostly due to numerics related to the surface boundary conditions. The commonly-used choice of $k-\varepsilon$ and Canuto A stability functions, however, appears to perform well in all test cases. The model performance is also strongly dependent on the chosen parameters which can be tuned in applications. For example, vertical profiles in the bottom friction test are affected by the choice of $c_\mu^0$ and $\sigma_\phi$ parameters, among others. Similarly, the length of salinity intrusion in the idealized estuary test case (Figure 6) depends on the magnitude of total

Figure 11: Evolution of surface salinity in the Columbia River application. The plotted stations are rino (▲), rice (♦), ogi01 (◉).
mixing which is partially controlled by the minimum value of TKE, $k_{min}$. Evidently, the parameters could be tuned further to reduce the gap between different closure models, for example. However, such an investigation of the parameter space is out of the scope of the present study.

The Columbia River plume simulation indicates that Thetis can represent tidal, highly dynamic river plumes. Comparison against SELFE also shows that lower numerical mixing in Thetis greatly improves the representation of the plume: There are strong frontal features which are retained over several tidal cycles. Numerous eddies and filaments are visible, and the plume responds quickly to changing tidal and wind conditions. In SELFE, on the other hand, numerical mixing results in a smoother and less dynamic mid-
and far-field plume. Excessive numerical mixing has been reported to destroy frontal features in the estuary (Kärnä et al., 2015; Kärnä and Baptista, 2016a). In this work, the diffused effect on the plume is evident both in the time series comparison (Figure 10 a) and the surface salinity fields (Figure 12). Overall, the results emphasize the importance of controlled numerical mixing in coastal ocean modeling.

The presented model uses $P^0_{DG}$ function space for the turbulent quantities while the mean flow values are in $P^1_{DG}$ space. This choice resembles the staggered discretization used in finite volume models (e.g. in GOTM) where the mean flow and turbulent variables are defined at cell centers and cell interfaces, respectively. As the turbulent quantities reside in a lower-degree function space, it could impact the accuracy of the coupled model. However, as the turbulence closure model only affects the mean flow model through the eddy viscosity and diffusivity fields, the impact is likely to be small. Deriving a higher-order discretization for the turbulent quantities remains a topic for future research.

6. Conclusions

We have presented a DG finite element discretization for the GLS turbulence closure model and a positivity-preserving coupled time integration scheme. The turbulence closure model was implemented in the Thetis circulation model.

The model was tested with a series of idealized test cases. The results verify that bottom boundary layer, surface mixing, and estuarine circulation processes are simulated correctly. All the three closures ($k-\varepsilon$, $k-\omega$, and GLS) and stability functions (Canuto A, B, and Cheng) yield similar performance.

Finally, the model was tested in a realistic Columbia River plume application. The results indicate that the coupled model performs well in complex, highly dynamic plume applications. The surface salinity values are in good agreement with observations. The simulated plume is relatively thin and rapidly responds to changing wind forcing. Compared to the SELFE model, the plume shows strong frontal features and eddies which suggests substantially lower numerical diffusion. Thetis, therefore, can retain fronts between water masses and capture the observed plume traversals with better skill.

There is an ever-increasing need for accurate, less dissipative coastal ocean models that can simulate buoyancy-driven coastal flows with a realistic rep-
representation of frontal features and vertical mixing. As such, the presented coupled circulation-turbulence model constitutes an important step towards next-generation ocean modelling.

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Appendix A. Source code availability

The source code used to perform the experiments in this paper is publicly available. Firedrake, and its components, may be obtained from https://www.firedrakeproject.org/ (last access: 10 July 2019); Thetis from http://thetisproject.org/ (last access: 10 July 2019). For reproducibility, we also cite archives of the exact software versions used to produce the results in this paper. All major Firedrake components and the Thetis source code have been archived on Zenodo zenodo/Firedrake, 2019; zenodo/Thetis, 2019.

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