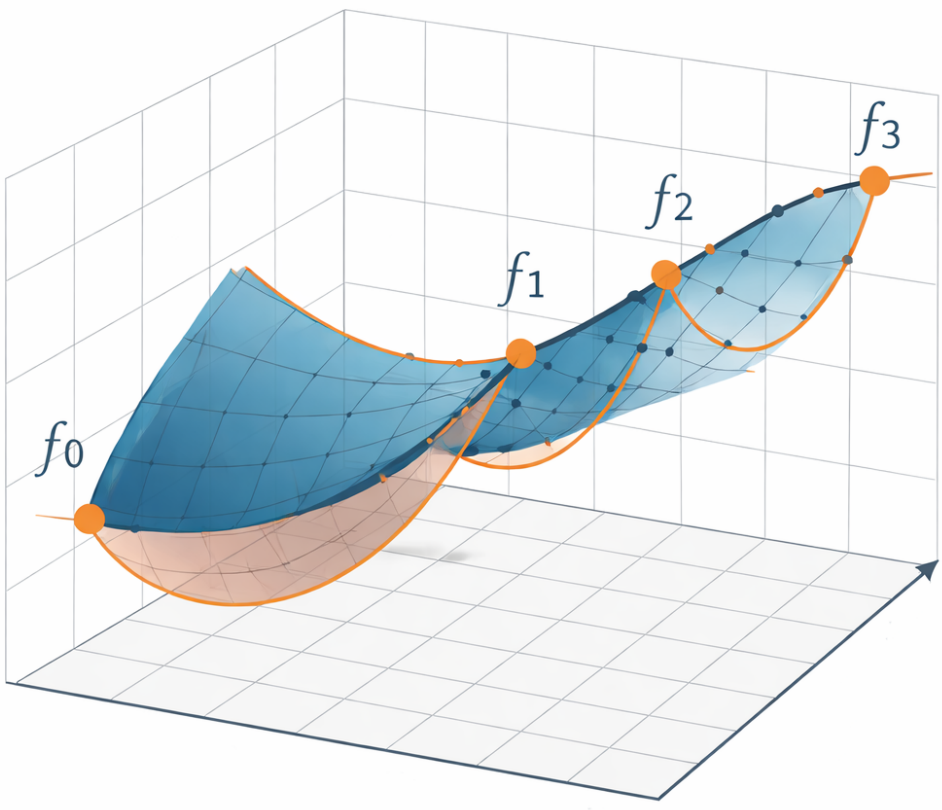
Implementation of ULTIMATE-QUICKEST for advective transport in EFDC+ White Paper

July 7, 2026



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Abstract

This white paper presents the integration of the ULTIMATE-QUICKEST numerical scheme into the Environmental Fluid Dynamics Code Plus (EFDC+) to enhance the simulation of advective transport of constituents. While the traditional upwind differencing method is robust, it introduces excessive numerical diffusion and can become computationally inefficient when correction terms are applied.

The proposed approach employs third-order quadratic interpolation combined with a specialized limiter, achieving higher spatial and temporal accuracy while preventing unphysical oscillations. Comparative tests across a range of 1D, 2D, and 3D models show that the new scheme more closely reproduces analytical solutions than conventional methods.

In addition, the implementation significantly improves computational efficiency, reducing total simulation runtimes by up to 30% in the Lake Mendota eutrophication model, with similarly substantial gains observed in other complex environmental applications.

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1 Introduction

The upwind differencing scheme implemented in EFDC+ is a robust method for solving the advective transport of constituents, as it ensures monotonic and bounded solutions. However, its first-order accuracy limits its ability to represent advective transport processes with high fidelity. Although the anti-diffusion correction has been implemented in EFDC+ to resolve unphysical oscillations at the expense of increased numerical diffusion the additional correction step reduces computational efficiency, in some cases significantly.

In fact, the limitations of the upwind scheme can be understood in terms of how wall (face) values of the dependent variables are estimated within a control-volume formulation. In the upwind approach, the face value is obtained through zeroth-order interpolation, with the upstream value selected according to the sign of the flow velocity. While this directional dependence provides strong numerical stability and convective sensitivity, the associated first-order truncation error introduces significant numerical diffusion, which can substantially degrade solution accuracy.

To address this limitation, the upcoming EEMS 12.5 release implements the QUICKEST scheme with the ULTIMATE limiter for the simulation of advective transport (Leonard, 1979, 1991). This approach employs consistent quadratic interpolation of the convective terms, achieving third-order accuracy in both space and time. Consequently, artificial diffusion is substantially reduced while numerical oscillations are effectively controlled. The following section presents a summary of the QUICKEST numerical algorithm and the ULTIMATE limiter. The corresponding implementation in EFDC+ is highlighted based on the approach described. Model results and computational performance using the QUICKEST scheme are then evaluated and discussed.

2 QUICKEST Numerical Algorithm

The QUICKEST algorithm (Quadratic Upstream Interpolation for Convective Kinematics with Estimated Streaming Terms) is based on a conservative control-volume formulation, developed by Leonard (1991) for unsteady flow which are primarily convective. This section describes the three main components of QUICKEST algorithm including quadratic interpolation, time integration and the flux correction using a ULTIMATE limiter.

2.1 Quadratic interpolation for spatial discretization

Consider the differential equation:

$$\frac{\partial \phi}{\partial t} = -\frac{\partial u\phi}{\partial x} + \frac{\partial}{\partial x} + S \tag{1}$$

Together with appropriate initial and boundary conditions, this can be interpreted as an unsteady one-dimensional convection-diffusion equation for the scalar ϕ with a well-defined source term $S(\phi, x, t)$.

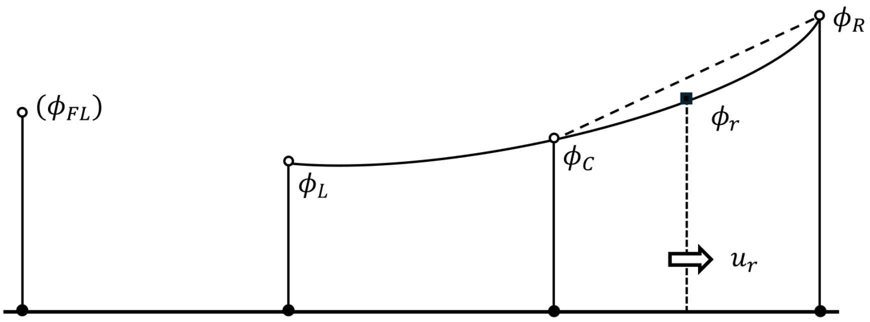

Figure 1: Quadratic upstream interpolation for ϕ_r and $(\frac{\partial \phi}{\partial x})_r$.

To construct an interpolation scheme which simultaneously possesses good accuracy and the directional properties associated with stable convective sensitivity, QUICKEST uses an asymmetrically placed three-point interpolation for each cell wall. The formulation of the QUICKEST algorithm is conveniently illustrated using constant grid spacing. Figure 1 shows the basic interpolation scheme for ϕ_r when u_r is positive to the right as shown. For steady flows, to calculate the value at a cell wall, the algorithm uses the two nodal values adjacent to the wall plus a third value from the next node upstream, i.e.:

$$\phi_r = \frac{1}{2}(\phi_C + \phi_R) - \frac{1}{8}(\phi_L + \phi_R - 2\phi_C) \tag{2}$$

which can be interpreted as a linear interpolation corrected by a term proportional to the upstream-weighted curvature. For modeling the gradient $\frac{\partial \phi}{\partial x_r}$, the tangent at the wall has also been shown in Figure 1. It is a geometric property of the parabola that the slope halfway between two points is equal to that of the chord joining the points, i.e.:

$$(\frac{\partial \phi}{\partial x})_r = \frac{\phi_R - \phi_C}{\Delta x_r} \tag{3}$$

which is valid in the variable-grid case as well, as indicated by the notation. This, of course, is identical to the central difference formula.

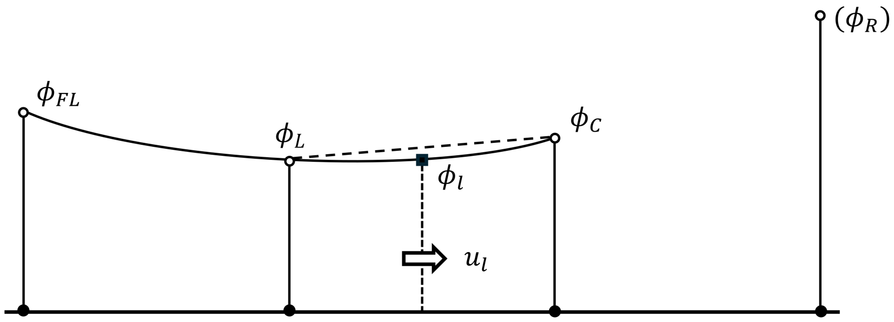

Figure 2: Quadratic upstream interpolation for ϕ_l and $(\frac{\partial \phi}{\partial x})_l$.

Similarly, Figure 2 shows the construction for ϕ_l and $(\frac{\partial \phi}{\partial x})_l$ when u_l, is also positive to the right. The corresponding formulas are:

$$\phi_l = \frac{1}{2}(\phi_L + \phi_C) - \frac{1}{8}(\phi_{FL} + \phi_C - 2\phi_L) \tag{4}$$

and:

$$\frac{\partial \phi}{\partial x_l} = \frac{\phi_C - \phi_L}{\Delta x_l} \tag{5}$$

The formulas 2-5 are appropriate to steady or quasi-steady flow in which Peclet number (P_Δ) is large in not more than one direction.

2.2 Time integration including estimated streaming terms

QUICKEST uses an explicit forward time-differencing approach. The general discretized transport equation for a node (i) is written as:

$$\frac{\phi_i^{n+1} - \phi_i^n}{\Delta t} = \frac{u_l \phi_l - u_r \phi_r}{\Delta x} + \text{Diffusion Terms} \tag{6}$$

where ϕ_l and ϕ_r are the time-average wall values.

The algorithm integrates this moving quadratic profile over the distance $u\Delta t$ to find the time-averaged wall value. This integration results in additional terms in the final formula that includes the Courant number $c = u\Delta t/\Delta x$ and the diffusion parameter $\alpha = \Gamma \Delta t/\Delta x^2$, ensuring the interpolation remains third-order accurate in both space and time. For a cell (i) with constant grid spacing (Δx) and velocity $u > 0$, the formula for the time-averaged value at the right cell wall ϕ_r is defined as:

$$\phi_r = \frac{1}{2}(\phi_C^n + \phi_R^n) - \frac{\Delta x}{2} c\,\text{GRAD}_r + \frac{\Delta x^2}{2}\left[\alpha - \frac{1}{2}(1 - c^2)\right]\text{CURV}_r \tag{7}$$

Where the spatial gradient at the wall, modeled as:

$$\text{GRAD}_r = \frac{\phi_R - \phi_C}{\Delta x} \tag{8}$$

And the upstream-weighted curvature, which provides the scheme its stability and high accuracy:

$$\text{CURV}_r = \frac{\phi_L + \phi_R - 2\phi_C}{\Delta x^2} \tag{9}$$

It is noted that the inclusion of terms involving the Courant number (c) represents the "Estimated Streaming Terms" (the EST in QUICKEST), which prevents the artificial numerical diffusion that occurs when using simpler unsteady schemes like upstream differencing.

2.3 Flux Correction using ULTIMATE limiter

Despite its accuracy, the QUICKEST scheme is still prone to unphysical overshoots and undershoots (numerical oscillations) when there are sharp changes in concentration gradients in purely advective flows. Therefore, the ULTIMATE algorithm is applied to the cell face values of the advection scheme to ensure they are "monotonized" and free of unphysical oscillations (Leonard, 1991). Rather than a single equation, the algorithm consists of a series of normalized variable definitions and limiting conditions.

To determine if a solution is monotonic, the algorithm first introduces normalized variables for each cell face. For a cell (i) and positive flow, the normalized concentration at the cell center and the right face are defined as:

$$\phi_i^n = \frac{\phi_i^n - \phi_{i-1}^n}{\phi_{i+1}^n - \phi_{i-1}^n} \tag{10}$$

And:

$$\phi_R = \frac{\phi_R - \phi_{i-1}^n}{\phi_{i+1}^n - \phi_{i-1}^n} \tag{11}$$

The algorithm checks if the unadjusted face value satisfies specific conditions to remain oscillation-free.

$$\text{if} \begin{cases} \phi_R \leq \phi_i^n & \text{for } 0 < \phi_i^n \leq 1 \\ \phi_i^n \leq \phi_R \leq 1 & \text{for } 0 < \phi_i^n \leq 1 \\ \phi_i^n = \phi_R & \text{for } \phi_i^n \leq 0 \text{ or } \phi_i^n > 1 \end{cases} \tag{12}$$

If these conditions are not met, then ϕ_R is adjusted to force a monotonic solution. The final, limited concentration value for the face is then reconstructed using the following formula:

$$\phi_R = \phi_{i-1}^n + \phi_R(\phi_{i+1}^n - \phi_{i-1}^n) \tag{13}$$

3 Code Implementation

EFDC+ solves the constituent transport equation through the subroutine **calconc**, which accounts for both advective and diffusive processes. Advective transport using the upwind scheme is handled by the subroutine caltran.

To incorporate the ULTIMATE-QUICKEST algorithm, a new subroutine, **caltran_quickest**, was developed to complement the existing **caltran** routine. This new routine applies the QUICKEST scheme for advective transport. In addition, the function **QUICKEST_FACE** was implemented to compute face concentrations using a third-order QUICKEST formulation, combined with the ULTIMATE limiter to ensure monotonicity and prevent spurious oscillations. Figure 3 summarizes the flowchart of the ULTIMATE-QUICKEST algorithm implemented in EFDC+. In contrast to the upwind scheme, which requires anti-diffusion corrections to improve accuracy, the QUICKEST approach achieves higher accuracy inherently while maintaining numerical stability.

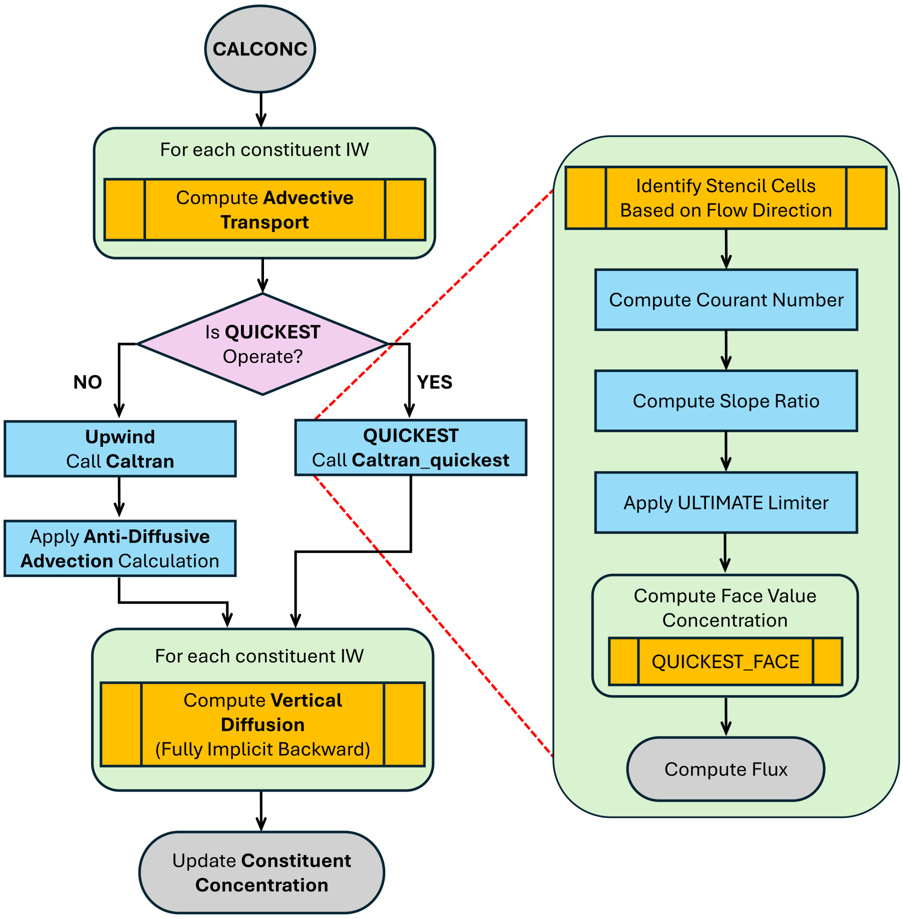

Figure 3: Implementation Scheme of QUICKEST algorithm in EFDC+.

4 First Tests Results

To demonstrate the practical advantages of the method over the existing upwind differencing scheme, we first perform several test-cases in comparison with available analytical solutions.

4.1 Chapra Anti-Diffusion

The Chapra Anti-Diffusion problem considers a rectangular 1D channel with a length of 5000 m and a width of 10 m. A conservative tracer with a constant concentration of 100 mg/L is introduced into the stream through an upstream inflow of 2 m^3/s. Figure 4 illustrates the model geometry, the locations of the boundary conditions, and the distribution of the tracer during the simulation. The horizontal domain is discretized using a uniform grid of 1 $\times$ 100 cells, each with a resolution of 50 m $\times$ 10 m. A single layer is used for the vertical discretization. The diffusion coefficient is set to 5 m^2/s. The objective is to replicate the test case for studying diffusivity effects on parameters outlined by Stephen C. Chapra in his book "Surface Water-Quality Modeling" for Distributed Series (Chapra, 1997).

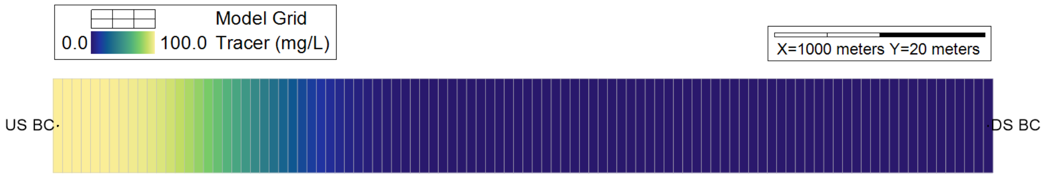

Figure 4: Chapra Anti-Diffusion: Model geometric configuration.

To verify the performance of the implemented QUICKEST algorithm, three model runs were conducted using three different numerical options for constituent advective transport in EFDC+, as follows:

- Run01 – Upwind Difference
- Run02 – Upwind Difference and Anti-Diffusion Correction and Flux Limitation
- Run03 – ULTIMATE-QUICKEST

Figure 5 compares the time evolution of tracer concentration at a point located 2000 m downstream for numerical and analytical solutions. The results show that the ULTIMATE–QUICKEST scheme and the Upwind scheme with Anti-Diffusion Correction produce similar results and closely match the analytical solution, whereas noticeable discrepancies occur when the Upwind scheme is used alone. These deviations originate from the inherent numerical diffusion associated with the first-order upwind differencing scheme. In EFDC+, this issue can be mitigated by enabling the Anti-Diffusion Correction option; however, this improvement comes at the cost of increased computational time. The impact of this additional computational cost will be further demonstrated in section 5 of computational efficiency.

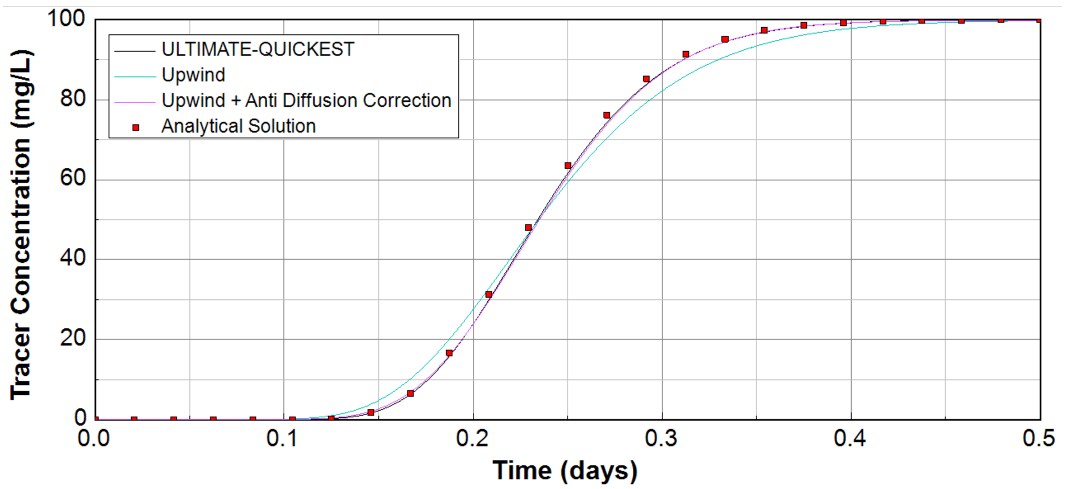

Figure 5: Comparison of tracer concentration time evolution.

The effect of Peclet number P_Δ, which represents the relative importance of advection and diffusion, was also investigated. This number is defined as:

$$P_\Delta = -\frac{u_0 \Delta x}{\Gamma_0} \tag{14}$$

in which, u_0 is the water velocity, Δx is the grid size, and Γ_0 is the diffusion coefficient.

In the previous model runs, with the diffusion coefficient set to 5 m^2/s, the resulting Péclet number was 1. To examine conditions where advection dominates, three additional model runs were conducted with the diffusion coefficient reduced to m^2/s, yielding a Péclet number of 5, indicating that advective transport becomes the dominant process. The comparison of the time evolution of tracer concentration at a point located 2000 m downstream between the numerical and analytical solutions is shown in Figure 6. The results indicate that the Upwind scheme with Anti-Diffusion Correction no longer matches the analytical solution under these conditions, whereas the QUICKEST scheme continues to provide good agreement with the analytical solution.

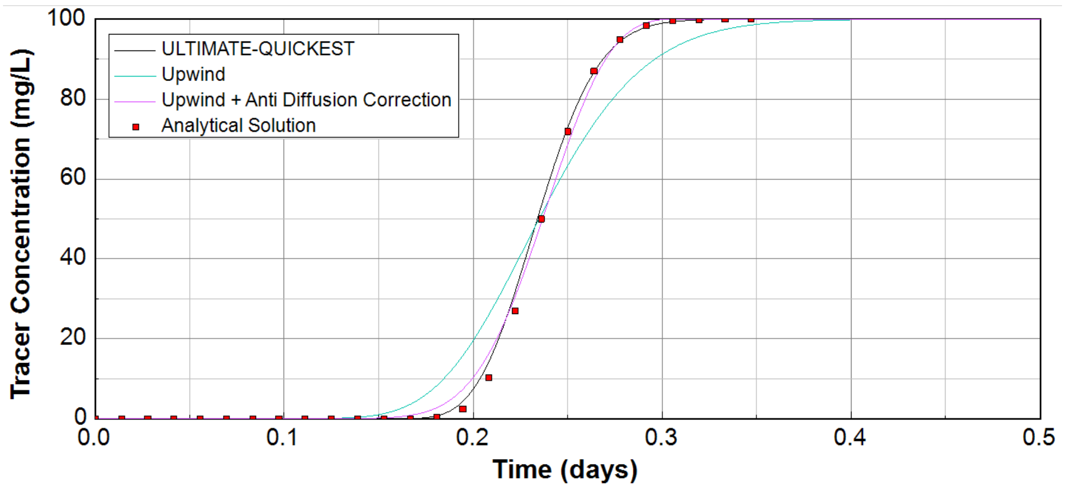

Figure 6: Comparison of tracer concentration time evolution for $P_\Delta = 5$.

4.2 Point-Hope

The 2D Point Hope model is second type of model problem to be considered demonstrates the practical advantages of the QUICKEST algorithm for unsteady flows which are primarily convective. Point Hope is located on the tip of the Tigara Peninsula on the northwest coast of Alaska, projecting into the Chukchi Sea. The hydrodynamic environment in this region is influenced by Pacific water inflow, wind forcing, weak tides, and seasonal sea-ice processes.

Figure 7 illustrates the model geometry and the locations of the boundary conditions. The model domain is discretized into 2700 cells, with an average resolution of 173.8 m $\times$ 110.7 m. The simulation scenario represents the dilution of a tracer initially and uniformly distributed in the water body at a concentration of 100 mg/L, driven by tidal exchange and outflow. The simulation period spans 10 days.

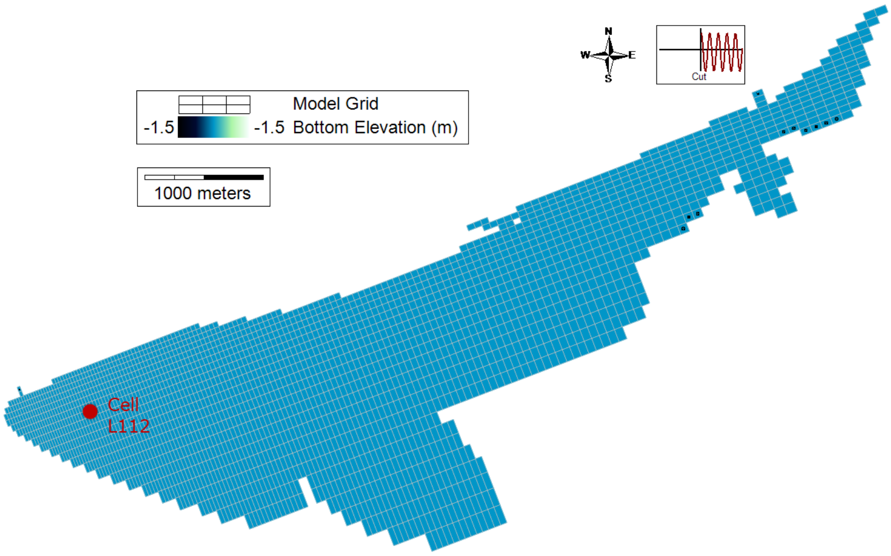

Figure 7: Point Hope Model - Geometry Configuration.

To verify the performance of the implemented QUICKEST algorithm, three model runs were conducted using different numerical options for constituent advective transport in EFDC+, as follows:

- Run01 – Upwind Difference and Anti-Diffusion Correction
- Run02 – Upwind Difference and Anti-Diffusion Correction and Flux Limitation
- Run03 – ULTIMATE-QUICKEST

Figure 8 present a comparison of the tracer concentration time series between three model runs at Cell 112, located at coordinates (X = 428.664 km; Y = 7583.983 km). The results indicate that Run01, which uses the Upwind scheme combined with Anti-Diffusion Correction option, exhibits an overshoot issue, with tracer concentrations exceeding 100 mg/L. The issue is also illustrated through the 2DH plan-view distributions of tracer on day 5 as shown in Figure 9. In contrast, the model Run02 when the additional Flux Limitation option is activated and the model Run03 using ULTIMATE–QUICKEST scheme do not exhibit the overshoot behavior.

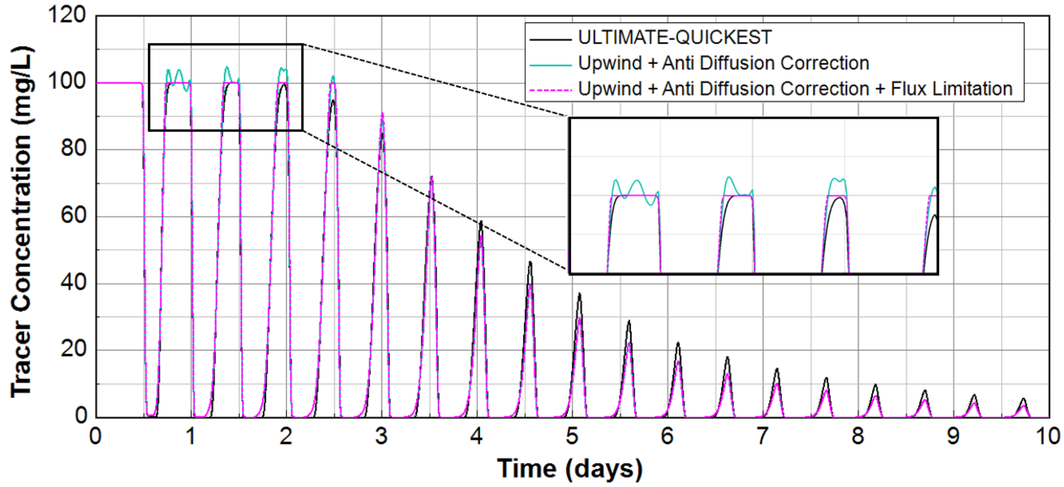

Figure 8: Point Hope Model - Comparison of tracer concentration time evolution between models Run01, Run01 and Run03.

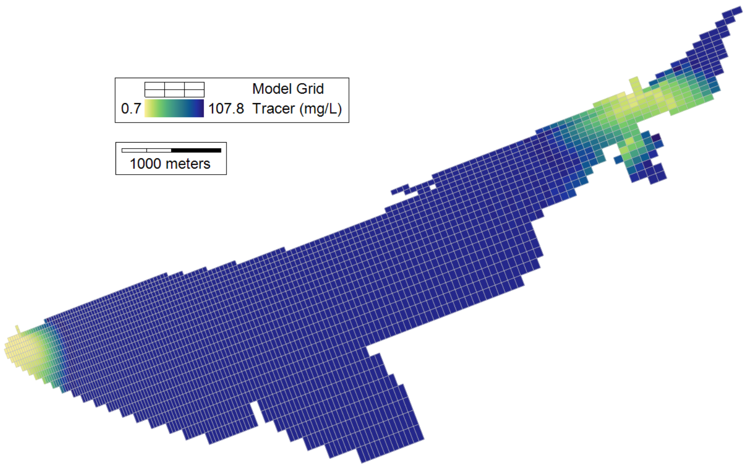

Figure 9: Point Hope Model - 2D Plan-view of Tracer concentration after 5 days by Run02 (Upwind Difference and Anti-Diffusion Correction).

5 Computational Performance Efficiency

To demonstrate the performance efficiency of ULTIMATE-QUICKEST over the upwind differencing scheme, we perform several real-world applications. For details, an application to a complex unsteady 3D Lake model also discussed to highlight the improved computational cost.

The 3D Lake Mendota Eutrophication model is the third type of model problem to be considered demonstrates the practical advantages of the QUICKEST algorithm, mainly focusing on the computation efficiency in real-world applications. Lake Mendota is a eutrophic freshwater lake located in Madison, Wisconsin, with a surface area of approximately 3,940 hectares. The lake has an average depth of 12.8 m, and its maximum depth reaches about 25.3 m. The primary hydrological inflows and outflows occur through the Yahara River. The phenomenon of eutrophication has been intensifying in Lake Mendota, leading to more frequent occurrences of harmful algal blooms. The decomposition of these blooms aggravates the anoxic conditions in the lake's deeper regions.

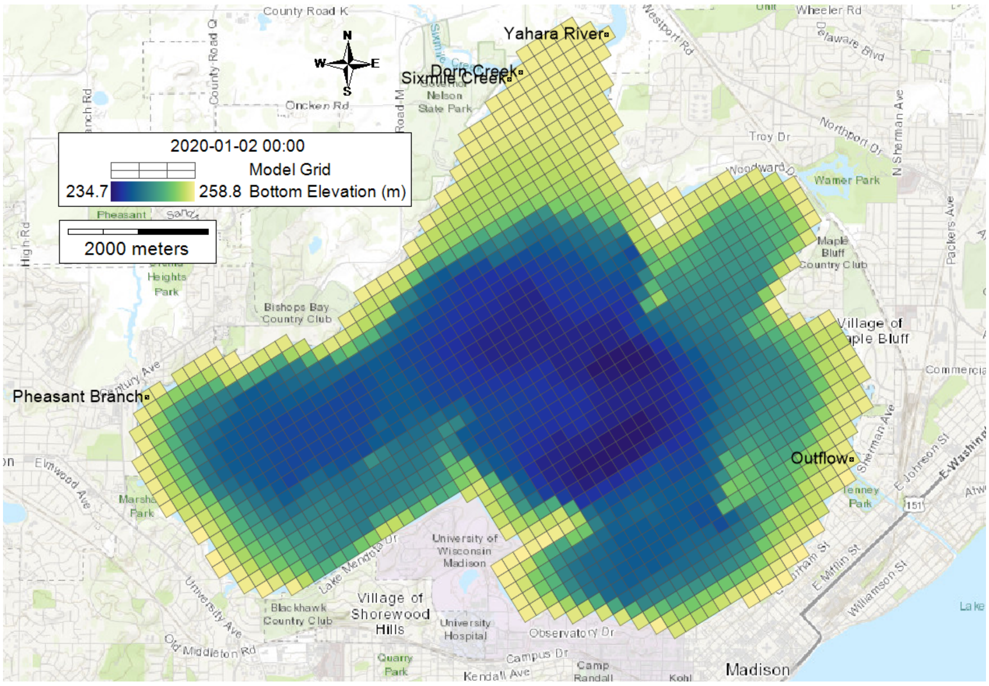

Figure 10: Lake Mendota Model Configuration

Figure 10 illustrates the model geometrical configuration, including the model grid, the locations of the boundary conditions, and the bottom elevation. The model domain is discretized using a uniform grid of 1405 cells, each with a resolution of 170 m × 170 m. The vertical layering uses SGZ uniform layers option varying from 3 to 30 layers.

The model simulates two algal groups: cyanobacteria and diatoms. Nutrient constituents Include organic carbon, nitrogen, phosphorus, and silica, each represented by their respective sub-classes: refractory particulate, labile particulate, and dissolved fractions. The total number of water quality constituents simulated is 18. The simulation covers a six-month period, from January 7, 2012, to December 28, 2012. Two model runs were conducted using the legacy upwind scheme implemented in EFDC+ and the new ULTIMATE-QUICKEST option, respectively:

- Run01 – Upwind Difference and Anti-Diffusion Correction and Flux Limitation.
- Run02 – ULTIMATE-QUICKEST

Figures 11 and 12 compare the numerical time series of temperature at different water depths at the BOUY point obtained from the two model runs. Minor differences between the Upwind and QUICKEST schemes are observed; however, overall, both schemes show good agreement with the observed data.

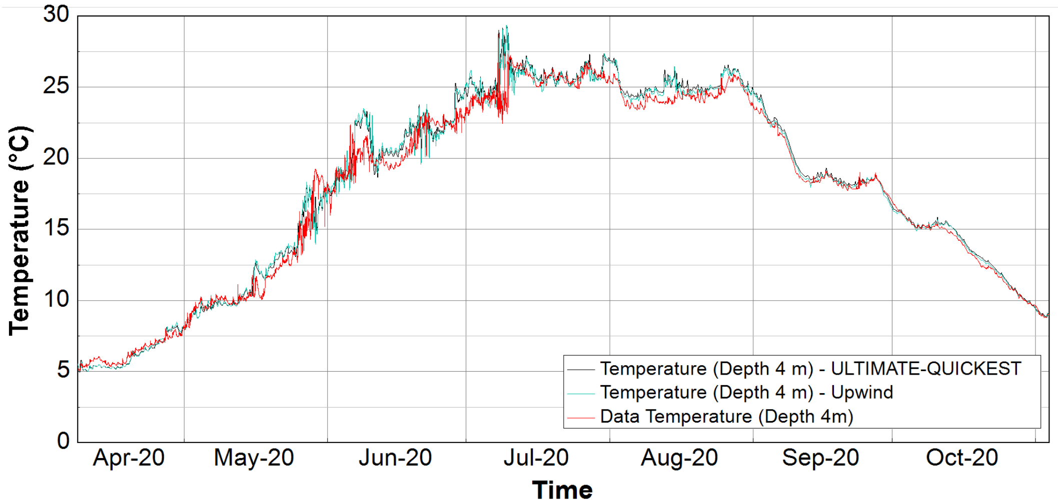

Figure 11: Comparison of temperature time series at BUOY point location at a depth of 4 m

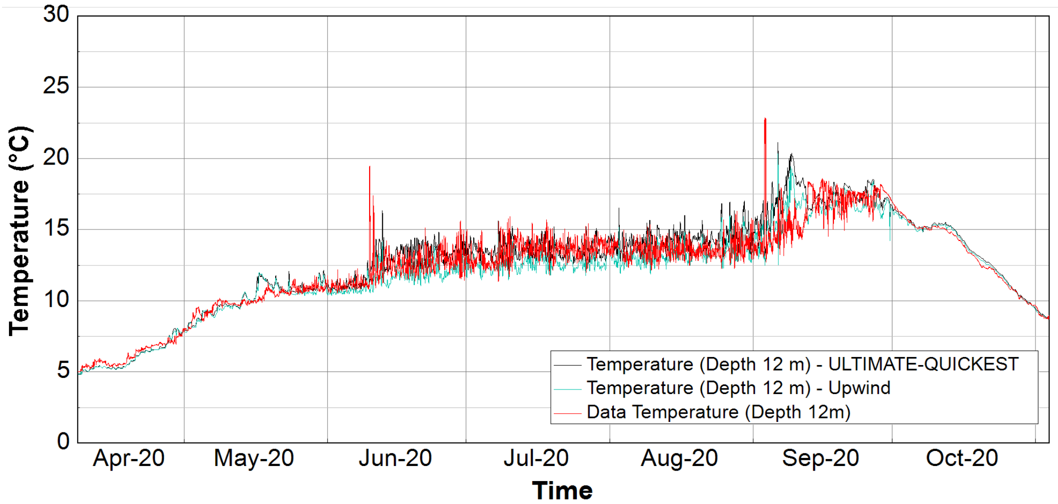

Figure 12: Comparison of temperature time series at BUOY point location at a depth of 12 m

Regarding computational efficiency, Figure 13 compares the total model run time and the time required for the advective transport process alone between the Upwind and QUICKEST schemes. The results show that the QUICKEST method significantly reduces the computation time for advective transport from 5.14 hours to 2.03 hours. This reduction contributes to an overall decrease in total model run time of over 30%.

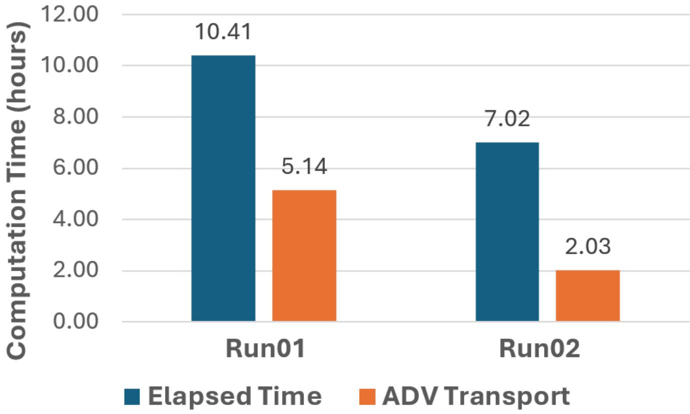

Figure 13: Comparison of computation time between Upwind and ULTIMATE-QUICKEST

Table 1 summarizes the computational cost improvements achieved by the ULTIMATE-QUICKEST scheme across different model applications. A significant reduction in computation time is observed in the advective transport calculations, contributing to a decrease in overall runtime. The efficiency gains become more pronounced as the number of simulated constituents increases. Additionally, 3D models exhibit greater reductions in computation time compared to 2D models, as they include advective transport in the vertical direction.

Table 1: Computation time reduced in different model applications

Model Name	Dim	Period	Consists	Elapsed Time (h)		ADV* Trans Time (h)		Reduction (%)	
				Upwind	Quickest	Upwind	Quickest	ADV	Total
Lake Mendota	3D	1 yr	19	10.41	7.02	5.14	2.03	60.5	32.6
Glenmore Reservoir	3D	1 yr	22	1.13	0.88	0.27	0.12	57.1	22.2
Lake Wash. Canal	3D	10 d	2	1.43	1.24	0.46	0.28	39.6	13.5
Bow River	2D	500 d	17	6.27	5.62	1.32	0.79	39.6	10.4
Portland Harbor	3D	6 mo	5	19.32	15.79	6.25	3.50	43.9	18.3

* Advective Transport

6 Conclusions

In this report, we present the implementation of the ULTIMATE–QUICKEST scheme for the advective transport of constituents in the EFDC+ code. The QUICKEST algorithm is described in terms of the quadratic interpolation used for spatial discretization, the time integration approach including estimated streaming terms, and the ULTIMATE limiter applied for flux correction.

The performance of the QUICKEST scheme is evaluated using three model problems, ranging from a simple 1D channel case to a 3D lake model. The results demonstrate that QUICKEST effectively reduces the numerical diffusion associated with the upwind differencing scheme, while also preventing unphysical overshoots and undershoots through the application of the ULTIMATE limiter. In addition, computational efficiency is improved, as the algorithm significantly reduces the time required for the advective transport calculations during the simulation.

References

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