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# Locally Filtered Transport for computational efficiency in multi-component advection-reaction models

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ABSTRACT

This work introduces the Locally Filtered Transport (LFT) method for numerical transport models. Locally turning off the transport computation in areas of nearly uniform concentration is proposed as a new approach for reducing computational cost in ecosystem models that require transport of tens to hundreds of constituent concentrations. The proposed method is locally mass conservative just as the discontinuous Galerkin finite element scheme it is based on. The performance of the method is illustrated using numerical examples including an advection-reaction ecosystem simulation with a simple nitrogen, phytoplankton, and zooplankton (NPZ) model.



## 1. Introduction

This work introduces and evaluates a new computationally-efficient scheme for transport equations in multi-component advection-diffusion-reaction models. The idea behind our method is quite simple: many physical, chemical, and biological processes take place on highly-localized spatial and temporal scales such that one or more transported constituents might be at quasi-uniform or "background" concentrations over large areas. For example, outside of a localized algae bloom, the *chlorophyll* concentration in a water quality model is typically at some background level, such that the same small concentration is fluxed in and out of most computational cells. These computational cycles of the transport equations are wasted and cannot affect the model results until the reaction equations initiate local growth of a bloom. Thus, an ecosystem model coupled to a large-scale circulation model (e.g., regional or global ocean, climate) incurs substantial computational costs for transport in parts of the spatio-temporal domain where some or all of the constituents are not present, have only the background concentration, or do not play a significant role in the reactions. For simple ecosystem models implemented in only two dimensions (2D), such as the Nitrogen-Phytoplankton-Zooplankton (NPZ) model used herein for demonstration purposes, the increased computational costs of transporting a few scalars is generally irrelevant. However, for ecosystem models that transport different species of plankton and include chemical speciation ($NO_3$, $NH_4$, dissolved inorganic carbon, dissolved organic carbon, etc.) the number of transported variables can easily be several dozen or more [e.g.Robson and Hamilton, 2004, Schwalb et al., 2015]. In three dimensions (3D) the extensive scalar transport requirements can dominate the overall computational time. Arguably, such models are computationally inefficient as they are not generally designed to identify and transport constituents only when and where they are significant. In this study, we demonstrate how to add such capability to an existing hydrodynamic/transport model with an approach we call Locally Filtered Transport (LFT).

We propose the new LFT algorithm that adaptively turns on/off the computation of certain discrete terms. The model performance

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is evaluated using a conventional (hydrostatic, inviscid) 2D shallow water and transport model based on the discontinuous Galerkin (DG) finite element method (Aizinger, 2004; Aizinger and Dawson, 2002). The present work builds on the background filtering approach (Hodges, 2014), which required an unconventional mass transport algorithm. Herein, we show that localization techniques can be efficiently extended to standard concentration transport schemes. Furthermore, the computational costs associated with localization that were identified in (Hodges, 2014) are elegantly handled within the DG framework using the vertex-based slope limiter (Aizinger, 2011; Kuzmin, 2010). The utility of the proposed approach is not limited to discontinuous Galerkin methods or geophysical applications: it can be easily transferred to any numerical PDE (partial differential equation) solver containing transport equations and might achieve meaningful performance gains even in the absence of reaction terms or in situations when only a few species are transported.

This paper is structured as follows. The system of governing equations is introduced in Sec. 2 followed by a description of the LFT method in Sec. 3. An NPZ ecosystem model is presented in Sec. 4, which is used as a test case for the LFT method combined with a DG hydrodynamic/transport model in Sec. 5. For completeness and to allow others to build on the modeling approach, the details of DG discretization are provided in Appendix A. A brief discussion and conclusions section completes the paper.

## 2. Governing equations

The model problem for this study is the 2D shallow water equations in conservative form, eqs. (1) and (2) below, combined with a varying number of equations for advection-reaction, represented by eq. (3) below, and augmented – as needed – by the corresponding initial and boundary conditions.

$$\partial_t \xi + \nabla\cdot(\boldsymbol{u}\, H) = 0, \tag{1}$$

$$\partial_t(\boldsymbol{u}\, H) + \nabla\cdot(\boldsymbol{u}\otimes\boldsymbol{u}H) + g\, H\, \nabla\xi + f_c\, \boldsymbol{k}\times\boldsymbol{u}\, H + \tau_{bf}\, \boldsymbol{u}\, H = H\boldsymbol{F}, \tag{2}$$

$$\partial_t(c_m\, H) + \nabla\cdot(\boldsymbol{u}\, H\, c_m) = H\, R_m(c_1, \ldots, c_M) + HF_m,\ m = 1, \ldots, M. \tag{3}$$

The primary unknowns in eqs. (1)–(3) are the water surface elevation ($\xi$) measured from a uniform datum, the depth-integrated horizontal velocity vector $\boldsymbol{u}\, H = [U, V]^T$, and the depth-integrated concentrations of multiple transported species $c_m\, H$, $m = 1, \ldots, M$. Given a boundary condition of spatially-varying bathymetry elevation, $b(x, y)$, the auxiliary variable $H$ denotes the total water depth $\xi - b$. All equations are required to hold on some Lipschitz bounded 2D domain $\Omega$ and on time interval $(0, T_{\text{end}})$. Furthermore, $g$ denotes gravity, $f_c$ is the Coriolis coefficient, $\boldsymbol{k}$ is the vertical unit vector pointing upwards, $\tau_{bf}$ is the coefficient of the quadratic friction law, $\boldsymbol{F} = (F_x, F_y)$ lumps together the forcing terms in the momentum equation (e.g., tidal potential), and $F_m, R_m,\ m = 1, \ldots, M$ are the source/sink terms and reaction rates in advection-reaction equations, respectively. With the exception of the reaction terms, the model is very similar to (Aizinger and Dawson, 2002), where the DG method was proposed for the 2D shallow water equations combined with non-reactive species transport.

Equations (1) and (2) utilize three types of boundary conditions (land, river, open sea) denoted by $\Gamma_l \cup \Gamma_r \cup \Gamma_s = \partial\Omega$, respectively, while eq. (3) for constituent transport may have boundaries that are inflow, outflow, or wall (no-flow). In this work, a river boundary is always an inflow boundary, a land boundary is always a wall boundary, and open sea boundaries are dynamically switched between the in-/outflow modes depending on the flow direction. These conditions are presented formally in Table 1.

## 3. Locally Filtered Transport

The LFT method relies on definition of an individualized *active domain* for each transported constituent that is a subset of the total domain $\Omega$. Each active domain evolves over time as advection-diffusion and reactions change the constituent concentration. Outside of the active domain the advection terms are ignored.

We consider two cases: first, as discussed in the introduction, there are regions of a computational domain over which some constituent might fall below a dynamically-meaningful concentration and may safely be ignored. Second, there is the possibility of regions with nearly uniform concentrations where transport is merely moving the same concentration about with no effect on the local distribution. For example, far away from the influence of estuaries, a large-scale ocean model that is not resolving salinity effects for meso-scale features might be simply shuffling around minuscule changes in salinity over the majority of the domain. A modeler might want to retain salinity transport for estuarine input to the coastal shelf, but it could be safely excised from the majority of the domain. Both cases can be addressed by monitoring the local concentration difference. Herein we define a *uniformity difference*, or $\delta_u$ for each constituent such that concentration differences between two neighboring grid elements smaller than $\delta_u$ allow the concentration to be considered locally uniform so that no transport computation is needed.

This general idea was introduced in (Hodges, 2014) as part of an algorithm using mass transport (rather than concentration transport) to allow local subtime stepping in regions where high velocities strictly limit the local advective time step. The prior methods had relatively high computational costs due to the approach taken to identify the active domain. In the present work, we adapt the background filtering from (Hodges, 2014) to the DG algorithm using uniform time steps and a conventional concentration transport discretization. Although the LFT idea can be extended to any model, the slope-limiting DG method (Aizinger, 2011; Kuzmin, 2010) has a particular advantage in that the majority of the computational effort for localization is already required in the existing transport algorithm, namely by the slope-limiting function (see Appendix A.5), which identifies and sorts the local concentration differences to maintain monotonicity.

The discrete time advance of eq. (3) for constituent transport is described in detail in Appendix A.5. For purposes of the LFT method, the key point is that the advance from time level $t^n$ to $t^{n+1}$ uses an explicit Runge-Kutta scheme with a slope limiter. At time $t^n$, the minimum and maximum values of a transported constituent for each computational element ($T_k$) that is connected to a node ($x_i$) are known from the slope limiter of the time advance from the $n-1$ to $n$ step, i.e. $a_i^{\min}$ and $a_i^{\max}$ are already defined at each vertex, see eq. (A.9). We use this time-lagged data to find the maximum nodal jump of scalar field $a$ for element $T_k$ and its nodal neighbors as

**Table 1**
Boundary conditions overview. Subscript $D$ indicates prescribed values of the variable, $\boldsymbol{\nu}$ denotes an exterior unit normal to the domain boundary.

| BC type | Shallow water | Transport |
|---|---|---|
| land $\Gamma_l$ | $\boldsymbol{u}\cdot\boldsymbol{\nu} = 0$ | $\boldsymbol{u}\cdot\boldsymbol{\nu}\, c_m = 0$ |
| river $\Gamma_r$ | $H = H_D,\ \boldsymbol{u} = \boldsymbol{u}_D$ | $c_m = (c_m)_D$ |
| open sea $\Gamma_s$ | $H = H_D$ | $c_m = (c_m)_D$ if $\boldsymbol{u}\cdot\boldsymbol{\nu} < 0$ |