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Gillibrand, Philip; Herzfeld, M.

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A Mass-Conserving Advection Scheme for Offline Simulation of Scalar Transport in Coastal Ocean Models

P.A. Gillibrand¹*, M. Herzfeld²

¹ Environmental Research Institute, North Highland College, University of the Highlands and Islands, Thurso, KW14 7EE, U.K.
² CSIRO Division of Marine and Atmospheric Research, GPO Box 1538, Hobart, Tas. 7001, Australia

* Corresponding Author.

Centre for Energy and the Environment
Environmental Research Institute,
North Highland College UHI,
Thurso, KW14 7EE,
U.K.

Tel.: +44 (0)1847 889686
Fax.: +44 (0)1847 889001
email: philip.gillibrand@uhi.ac.uk

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Abstract

We present a flux-form semi-Lagrangian (FFSL) advection scheme designed for offline scalar transport simulation with coastal ocean models using curvilinear horizontal coordinates. The scheme conserves mass, overcoming problems of mass conservation typically experienced with offline transport models, and permits long time steps (relative to the Courant number) to be used by the offline model. These attributes make the method attractive for offline simulation of tracers in biogeochemical or sediment transport models using archived flow fields from hydrodynamic models. We describe the FFSL scheme, and test it on two idealised domains and one real domain, the Great Barrier Reef in Australia. For comparison, we also include simulations using a traditional semi-Lagrangian advection scheme for the offline simulations. We compare tracer distributions predicted by the offline FFSL transport scheme with those predicted by the original hydrodynamic model, assess the conservation of mass in all cases and contrast the computational efficiency of the schemes. We find that the FFSL scheme produced very good agreement with the distributions of tracer predicted by the hydrodynamic model, and conserved mass with an error of a fraction of one percent. In terms of computational speed, the FFSL scheme was comparable with the semi-Lagrangian method and an order of magnitude faster than the full hydrodynamic model, even when the latter ran in parallel on multiple cores. The FFSL scheme presented here therefore offers a viable mass-conserving and computationally-efficient alternative to traditional semi-Lagrangian schemes for offline scalar transport simulation in coastal models.

Keywords: tracer; advection; transport; semi-Lagrangian; coastal ocean model; mass conservation.
1. Introduction.

Transport models that provide the solution to the advection-diffusion equation for tracers using offline flow data are popular due to the potential increase in execution speeds of several orders of magnitude. These types of models have been used in atmospheric chemistry models for some time (Rood, 1987), but have yet to be entrenched in the ocean modelling community. Decreased run-time becomes particularly important when using benthic-pelagic biogeochemical models that utilize many tracers (e.g. Wild-Allen et al., 2013), since the execution times of these models when fully coupled to hydrodynamic models is typically an order of magnitude more than the hydrodynamic model in isolation. There are, however, several issues with the offline transport model approach; firstly storage space for the flow data can be prohibitive for long simulations, and secondly conservation of the tracer fields is difficult to ensure. The former issue may be addressed by using unstructured coordinate systems (e.g. Herzfeld 2006) where non-wet cells (land cells, those beneath the sea bed) can be omitted when writing to file. This can achieve up to 90% reduction in file size, depending on the domain simulated. More recently, the use of compression with netCDF4 can achieve a similar result. The latter problem has been considered by numerous studies (e.g. Dawson et al. 2004; Naifar et al. 2007), and can be avoided if the schemes used to compute the flow and tracer transport are compatible. Compatibility, or consistency, in this context is defined by Gross et al. (2002) as: ‘A discretization of the advection equation is consistent with continuity if, given a spatially uniform scalar field as an initial datum, and a general flow field, the discretized scalar advection equation reduces to the discretized continuity equation.’ In order to ensure conservation, the transport algorithm must satisfy the constancy condition (Naifar et al, 2007), where in the absence of sources or sinks, an initially uniform tracer field remains uniform thereafter. A consistent transport discretization is sufficient to satisfy the constancy condition (Lin and Rood, 1996; hereafter LR96).

If a different offline numerical scheme is used to compute the transport than that used to compute the flow, the consistency condition is often not maintained leading to spurious fluxes (LR96). Naifar et al (2007) report that in order to satisfy the constancy condition in the transport solver, the flow fields have to satisfy the continuity equation up to machine accuracy. These authors achieved this by adjusting surface heights at each time step so that continuity is exactly satisfied. LR96 noted that for atmospheric transport models, although winds satisfy the continuity equation in the wind producing model, they are in general not consistent with the discrete form of the tracer equation. The flow field in the transport model can be adjusted to enforce continuity (e.g. Deleersnijder, 2001), although this may result in unacceptable velocities (Allen et al. 1991), or a correction can be added to the transport scheme to compensate for a non-conservative velocity field (Dawson, 2000). Generally, inconsistency is addressed by two methods: either selecting flow and transport schemes that are consistent with each other, or by applying corrections (Naifar et al,

The time-scales involved in biogeochemical processes are also typically longer than that of the associated hydrodynamics, and it is advantageous to exploit this by using a longer time-step for the transport algorithm. This is essential in order to achieve speed-ups of several orders of magnitude, and an unconditionally stable semi-Lagrangian advection scheme may be used to achieve this. Since these schemes are discretized from the advective form of the tracer conservation equation, they are globally and locally non-conservative. Furthermore, the flow fields used in the transport model may often derive from hydrodynamic models where the output was not stored with the view to subsequent use in a transport model. For example, global models are often run for the purpose of examining physical processes in the ocean or climate change, and flow fields are typically saved as daily means or snapshots. The storage required to dump output from these global models at higher frequency is prohibitive. However, it may be desirable to use these outputs to generate global or regional biogeochemical models. Since the time integral of a flow field and water depth will not necessarily satisfy the continuity equation when daily mean flow fields are used offline in a transport model, a non-conservative tracer solution results. Conservative semi-Lagrangian schemes whose time-step is limited to the Courant number < 1 (Incremental Re-mapping) have been described by Dukowicz and Baumgardner (2000) and Lipscomb and Ringler (2005). This restriction on the time-step was relaxed using cell-integrated semi-Lagrangian scheme in two dimensions (CISL, Nair and Machenhauer, 2002), although local conservation was not maintained near the poles on a spherical grid. Also, the time step must be such that trajectories or line segments of the grid do not cross in the backward streamline integration. Stable transport algorithms that are conservative do exist, e.g. non-interpolating schemes (Staniforth and Cote, 1991), flux-form semi-Lagrangian (LR96), the COSMIC scheme of Leonard et al. (1996) or finite volume approaches to the semi-Lagrangian scheme (Leslie and Purser, 1995, references in Nair et al (2003)). Bermejo (1990) also reported that semi-Lagrangian schemes using cubic spline interpolation conserve mass (for divergence-free flows). However, the use of daily- (or hourly-) mean flow data in these schemes may still result in a non-conservative solution due to violation of the constancy condition. An alternative approach to ensuring global mass conservation is the a posteriori restoration of mass (e.g. Priestly, 1993), also referred to as global filling (Rood, 1987).

Of particular interest here are the schemes of LR96 and Leonard et al. (1996) who both applied semi-Lagrangian techniques to the volume fluxes across cell faces, rather than to the cell-centred tracer itself; local tracer concentrations were then updated by solving the local mass balance. This approach ensured that local mass was conserved and, by extension, the domain-wide mass was also conserved. The use of semi-Lagrangian techniques to the volume fluxes allowed long (relative to the Courant number) time steps to be used. Both LR96 and Leonard et al. (1996) demonstrated the method on regular grids with constant grid spacing.
In this paper, we adapt the flux-form semi-Lagrangian (FFSL) scheme of LR96 and Leonard et al. (1996) to coastal ocean hydrodynamic and transport models, by developing their algorithm to apply on curvilinear coordinate grids with variable horizontal grid spacing, as are often used in coastal ocean models. Our motivation is to develop an advection scheme that may be used by offline coastal ocean ecological models, that allows long time steps (relative to the Courant restriction) for computational efficiency and that also conserves mass. In the following sections we describe the scheme, apply it to two idealized test domains and one real domain, and demonstrate that the FFSL scheme produces accurate and conservative tracer distributions compared to the original hydrodynamic model used to generate the flow fields. To illustrate the benefits of the approach, we also compare the FFSL results with a traditional semi-Lagrangian advection scheme, with and without global filling. We also compare the computational speeds of the various schemes.

2. Methods

2.1 The Flux-Form Semi-Lagrangian Scheme

We seek to solve the transport equation for a tracer $\varphi$ conservatively with the ability to use long ($C_t >> 1$) time steps, where $C_t = \max(u_1\Delta t/h_1, u_2\Delta t/h_2, w\Delta t/h_3)$ is the Courant number. From the prior hydrodynamic model simulation, the cell dimensions ($h_1, h_2, h_3$), instantaneous sea surface elevation $\eta_{i,j}^n$, time-averaged volume fluxes $(u_1^n h_1^2 h_3^{n+\frac{1}{2}})_{i\pm\frac{1}{2},j}$ and $(u_2^n h_2 h_3^{n+\frac{1}{2}})_{i,j\pm\frac{1}{2}}$, and the time-averaged vertical eddy diffusive fluxes are known at each time step (superscript $n$ of the offline scheme) and grid location $(i,j)$ on a staggered curvilinear Arakawa ‘C’ grid where $h_1$, $h_2$ and $h_3$ are not necessarily constant.

One of the keys to decreasing run-times in a scalar transport model is to increase the time step relative to the hydrodynamic model time step. However, the conservative semi-Lagrangian approaches cited above must use underlying flow and free-surface elevation fields that together conserve volume (e.g. Casulli and Zanoli, 2005) i.e. that satisfy the continuity equation which, for an incompressible fluid under hydrostatic conditions, is:

$$\frac{\partial \eta}{\partial t} + \nabla_H \cdot \left( \eta \bar{u} dz \right) = 0$$

(1)

where $\bar{u}$ is the three-dimensional velocity vector, $\nabla_H$ is the horizontal divergence operator and $z$ is the vertical coordinate. Satisfying Equation (1) with archived flow fields is generally only achievable when the time step used by the transport model is identical to that of the hydrodynamic model used to generate the flow fields. In most cases this is not desirable, as cost savings are then very limited. Using a longer time-step for transport, in conjunction with snapshots or temporal
averages of velocity and surface elevation fields, usually results in a failure to conserve volume. For a snapshot this is obvious; continuity is only achieved if the velocity is constant over the transport time-step, an unlikely circumstance. For temporal means of velocity, the change in elevation over the averaging time step is not necessarily equal to the divergence of average velocity multiplied by water depth, i.e. if a velocity mean is computed between \( t_1 \) and \( t_2 \), then

\[
\Delta \eta = \int_{t_1}^{t_2} \mathbf{d} \cdot \nabla H \int_{t_1}^{t_2} \mathbf{U} \cdot \mathbf{d} dt
\]

where \( D = \eta + H \) is the total water depth, \( H \) is the depth relative to \( \eta = 0 \), and \( \mathbf{U} \) is the depth-averaged velocity. However,

\[
\Delta \eta = -\nabla H \int_{t_1}^{t_2} D \mathbf{U} \cdot \mathbf{d} dt
\]

which suggests that a transport scheme that uses temporal averages of the volume fluxes rather than velocities will allow conservative solutions using time steps longer than that used in the underlying hydrodynamic model. This forms the basis of the flux form semi-Lagrangian scheme.

2.1.1 Mathematical Framework

The three-dimensional advection-diffusion transport equation for a scalar \( \phi \) in an incompressible fluid can be written:

\[
\frac{\partial \phi}{\partial t} + \nabla (\mathbf{u} \phi) = \frac{\partial}{\partial z} \left( K_z \frac{\partial \phi}{\partial z} \right)
\]

(2)

where \( K_z \) is the vertical eddy diffusivity. Implementing a flux-form solution on a curvilinear grid leads to:

\[
\frac{\partial (h_i \phi)}{\partial t} + \frac{1}{(h_i h_j)} \left[ \frac{\partial (u h_i h_j \phi)}{\partial \xi_1} + \frac{\partial (v h_i h_j \phi)}{\partial \xi_2} \right] + \frac{\partial (w h_i \phi)}{\partial z} = \frac{\partial}{\partial z} \left( K_z \frac{\partial (h_i \phi)}{\partial z} \right)
\]

(3)

where \( \xi_1 \) and \( \xi_2 \) are the horizontal coordinates on the grid.

Following the procedure described by Lin & Rood (1996), the updated tracer concentration at time step \( n+1 \), \( \phi^{n+1} \), is given by:
\[ \phi_{i,j}^{n+1} = \frac{1}{h_x^{n+1}} \left\{ (h_x \phi_{i,j})^{n} - F \left[ \phi^n + \frac{1}{2} g(\phi^n) \right] - G \left[ \phi^n + \frac{1}{2} f(\phi^n) \right] - H [\phi^n] \right\} \] (4)

where

\[
F[\theta] = \frac{1}{(h_1 h_2)_{i,j}} \left[ X_{i+\frac{1}{2},j} - X_{i-\frac{1}{2},j} \right] = \frac{1}{(h_1 h_2)_{i,j}} \left[ \Delta t (u_1 h_2 h_3 \theta)_{i+\frac{1}{2},j} - \Delta t (u_1 h_2 h_3 \theta)_{i-\frac{1}{2},j} \right]
\]

\[
G[\theta] = \frac{1}{(h_1 h_2)_{i,j}} \left[ Y_{i,j+\frac{1}{2}} - Y_{i,j-\frac{1}{2}} \right] = \frac{1}{(h_1 h_2)_{i,j}} \left[ \Delta t (u_2 h_1 h_3 \theta)_{i,j+\frac{1}{2}} - \Delta t (u_2 h_1 h_3 \theta)_{i,j-\frac{1}{2}} \right]
\]

\[
H[\theta] = Z_{k+\frac{1}{2},j} - Z_{k-\frac{1}{2},j} = \Delta t \left[ (w \theta)_{k+\frac{1}{2},j} - (w \theta)_{k-\frac{1}{2},j} \right]
\]

\[
f(\theta) = \left( \frac{u_1 \Delta t}{h_1} \right)_{i,j} \left[ \theta_{i+\frac{1}{2},j} - \theta_{i-\frac{1}{2},j} \right]
\]

\[
g(\theta) = \left( \frac{u_2 \Delta t}{h_2} \right)_{i,j} \left[ \theta_{i,j+\frac{1}{2}} - \theta_{i,j-\frac{1}{2}} \right]
\]

and

\[
u_{1i,j} = \frac{u_{1i+\frac{1}{2},j} + u_{1i-\frac{1}{2},j}}{2}
\]

\[
u_{2i,j} = \frac{u_{2i,j+\frac{1}{2}} + u_{2i,j-\frac{1}{2}}}{2}
\] (6)

The terms \( F[] \) and \( G[] \) denote the horizontal mass flux divergences in each direction, and \( H[] \) denotes the vertical divergence. The terms \( g(\phi) \) and \( f(\phi) \) are transverse advection terms that are required to improve accuracy and maintain numerical stability with the longer time step \( \Delta t \) that may be used (LR96; Leonard et al. 1996). The terms \( X, Y \) and \( Z \) are the mass transports at cell faces in the horizontal and vertical directions. Equation 4 is equivalent to equations 2.27 (2D transport equation) and 4.2 (3D transport equation) in LR96; the derivation of Equation 4 can therefore be obtained from that paper. The fundamental difference between Equations 4 and 5 and their equivalents in LR96 is that the cell dimensions \( (h_1, h_2, h_3) \) are retained here, because the cross-sectional areas of grid cells on curvilinear grids are variable, whereas in LR96 the constant grid size \( \Delta x \) means that cross-sectional cell areas are identical across the grid and the cell dimensions therefore drop out from the final mathematical expressions.

LR96 treat the vertical transport independently of the horizontal transport (in the sense that the transverse terms associated with vertical advection are ignored). In this case, two additional 3D tracers must be declared for each modelled tracer in order to calculate the transverse terms. For the
fully 3D COSMIC scheme of Leonard et al. (1996), the transverse terms are calculated in all three dimensions, leading to the calculation of an additional six tracers for each modelled tracer. Thus the FFSL scheme has the potential to be significantly quicker than the COSMIC scheme, but the COSMIC scheme is likely to be more stable numerically.

In order to allow long time steps, the flux terms, X, Y and Z, must be broken into integer and fractional components relative to the local grid spacing (Fig. 1). On grids with constant spacing, the integer component can be derived easily from the grid spacing (c.f. Equation 3.5 in LR96). On curvilinear grids, however, the integer component in the $\xi_1$ direction, for example, must be derived by tracing back along the $\xi_1$ trajectory component and subtracting successive values of $h_1$ from the trajectory length until the remainder of the trajectory is less than the next value of $h_1$. The integer number of grid cells within the trajectory for a cell face velocity $u_{i-\frac{1}{2},j}$ is denoted by $K_{i-\frac{1}{2}}$ (note that $K_{i+\frac{1}{2}}$ has the opposite sign to $u_{i+\frac{1}{2},j}$).

The integer flux at a left-hand face, $I_{i-\frac{1}{2}}$, is computed by:

$$I_{i-\frac{1}{2}}(\theta) = \begin{cases} \sum_{k=-i}^{i} \theta^n_{i-k}, & K_{i-\frac{1}{2}} \geq 1 \\ 0, & K_{i-\frac{1}{2}} = 0 \\ \sum_{k=i+1}^{i} \theta^n_{i+k}, & K_{i-\frac{1}{2}} \leq -1 \end{cases} \quad (7)$$

The fractional component of the $\xi_1$-direction trajectory $c_{i,\Delta x,j}$ is then expressed as the ratio of the remainder of the trajectory, $\delta x$, and $h_1$ at the head of the trajectory i.e.

$$c_{i-\frac{1}{2},j}^x = \begin{cases} \frac{\delta x_{i-\frac{1}{2}}}{h_{1+K_{i-\frac{1}{2}}}}, & u_{i-\frac{1}{2}} > 0 \\ 0, & u_{i-\frac{1}{2}} = 0 \\ \frac{\delta x_{i-\frac{1}{2}}}{h_{1+K_{i-\frac{1}{2}}}}, & u_{i-\frac{1}{2}} < 0 \end{cases} \quad (8)$$

Integer and fractional components of trajectories from both cell centres (Fig. 1a) and cell faces (Fig. 1b) must be calculated for both the $\xi_1$ and $\xi_2$ directions.
2.1.2 Implementation

The FFSL algorithm on curvilinear grids operates as follows. To solve the tracer flux in the $\xi_1$ direction, define a temporary tracer, $\phi_{i,j}^s$, that includes the transverse terms, such that:

$$
\phi_{i,j}^s = (\phi)_{i,j}^n + \frac{1}{2} g_{i,j}
$$

$$
= \frac{1}{2} \left[ \phi_{i,j}^n + \phi_{i,j}^* + \left| c_{i,j} \left( \phi_{i,j}^n - \phi_{i,j}^* \right) \right] \right]
$$

where the indices $J$ and $J^*$ are given by

$$
J = j - K_{i,j}^x
$$

$$
J^* = J - \text{SIGN}(1, K_{i,j}^x)
$$

Then define $\Phi^\prime = (h_i, \phi_{i,j}^s)^n_{i,j}$. The mass transport across the left-hand face of the cell $(i,j)$ is given by:

$$
X_{i-\frac{1}{2},j} = (h_i h_3)_{i-\frac{1}{2},j} I_{i-\frac{1}{2},j} (\Phi^\prime) + c_{i-\frac{1}{2},j} (h_i h_3)_{i-\frac{1}{2},j} \Phi_{i,j}^\prime
$$

$$
I = \text{INT}(i - C_{i-\frac{1}{2},j}^x)
$$

The terms $X_{i+\frac{1}{2},j}$, $Y_{i,j+\frac{1}{2}}$, $Y_{i,j+\frac{1}{2}}$, $Z_{k\frac{1}{2},j}$, $Z_{k\frac{1}{2},j}$, $Z_{k+\frac{1}{2}}$, are calculated similarly. From these terms, the updated tracer concentration at the cell centre can be derived.

From the prior hydrodynamic model simulation, instantaneous values of the sea surface height $\eta^n$ at set intervals (e.g. hourly) must be archived. The temporal-mean values of the volume fluxes [e.g. $(u_i h_i h_3)_{i+\frac{1}{2}}$] and velocities [e.g. $(u_i)_{i+\frac{1}{2}}$] at cell faces must be averaged over the interval between the instantaneous sea surface height values, thereby being centred at time step $n+\frac{1}{2}$. It is necessary to archive both velocity fluxes and velocities because the former are required for the flux calculations described above, and the latter are used to determine the trajectory distances.
2.1.3 Stability

The transport model described above is not unconditionally stable, but is subject to the Lipschitz condition (LR96):

$$\max \left( \frac{\Delta t \Delta u_1}{h_1}, \frac{\Delta t \Delta u_2}{h_2}, \frac{\Delta t \Delta w}{h_3} \right) \leq 1$$  \hspace{1cm} (12)

where $\Delta u_1$ etc are the differences between the velocities on the upstream and downstream faces of a cell i.e.

$$\Delta u_{i,j} = |u_{i+1/2,j} - u_{i-1/2,j}|$$  \hspace{1cm} (13)

The time step is set by calculating the values of $\Delta u_1/h_1$, $\Delta u_2/h_2$ and $\Delta w/h_3$ across the grid at each time step, and ensuring the above condition (12) is met.

The Lipschitz condition essentially ensures that streamlines emanating from adjacent cell faces do not cross, and is typically much less restrictive than the usual Courant number condition. However, the Lipschitz number is a function of the grid spacing ($h_1$), and will become more restrictive for higher resolution grids.

2.2 Traditional Semi-Lagrangian Scheme with Global Filling

Semi-lagrangian methods for simulating advection in geophysical fluids have been reviewed by Staniforth and Cote (1991). The implementation of our basic scheme follows the method described for an ocean model by Casulli and Cheng (1992), and the extension to the higher order scheme used in one test case follows McDonald (1984). Here, we describe the steps taken to ensure mass conservation with the traditional semi-Lagrangian scheme in our model.

The errors leading to non-conservation of mass in traditional semi-Lagrangian schemes using long time-steps can be summarised as follows:

(i) The semi-Lagrangian scheme is cast in advective form and is intrinsically non-conservative.

(ii) Continuity is not achieved when using snapshots or temporal averages of velocity and/or surface elevation over the long time-step.

In order to render the semi-Lagrangian advection scheme conservative, *a posteriori* restoration, or filling, of mass can be applied. This can be as simple as computing the total mass in
the domain before and after advection, and multiplicatively adjusting the mass after advection to ensure pre- and post-advection mass is identical. If open boundaries are present, then mass fluxes across the boundary are required to be added to the initial mass. Monotonicity must also be maintained, so that adjusted concentrations do not become greater or less than the local maxima or minima respectively at the streamline origin in the semi-Lagrangian method. This can be achieved by excluding mass filling at those locations where monotonicity is violated, and iteratively applying the multiplicative fill until all mass is accounted for. This mass filling approach has the effect of a local transfer of mass to the global domain, and can be considered ‘global filling’ (i.e. mass is still not conserved locally at a grid cell).

Estimating open boundary mass fluxes can be a source of error, since the tracer field required beyond the open boundary is not known, making interpolation of tracer values onto the boundary face uncertain. Volume calculation is not subject to errors from (i) above, so assuming volume (V) fluxes are due to n open boundaries (OBCn) the mass budget is:

\[ V^t + \sum_{n} OBC_n = V^{t+1} \]  

(14)

Any error from (ii) can be compensated by adjusting the boundary fluxes by some factor f:

\[ f = \frac{V^{t+1} - V^t}{\sum_{n} OBC_n} \]  

(15)

This ensures domain-wide volume divergence is equal to the change in volume within the domain over the time-step. This factor, f, may then be applied to mass fluxes for tracers in the transport model in an attempt to improve the boundary flux mass contribution. Implementation of open boundary conditions in the present model is described by Herzfeld and Andrewartha (2012) and Herzfeld and Gillibrand (2015).

In the tests described here, the semi-Lagrangian schemes predominantly used a tri-linear interpolation scheme, effectively rendering the advection scheme to 1st order which is characterized by high numerical diffusion. (An exception was for the GBR test case, for which a semi-Lagrangian scheme with a third order interpolation (McDonald, 1984) was also tested). For this reason, no explicit horizontal diffusion was implemented by the transport model. Vertical eddy diffusion was always included in the transport model simulations, with values taken from the hydrodynamic model data files.
2.3 The hydrodynamic model

The model used to test the advection scheme is described in Herzfeld (2006). This is a 3D finite difference model based on the study of Blumberg and Herring (1987). It utilizes an Arakawa C grid, uses a free surface, mode splitting and partial bottom cells. The model is based on the equations of momentum, continuity and conservation of heat and salt, employing the hydrostatic and Boussinesq assumptions. An orthogonal curvilinear grid is used in the horizontal and wetting and drying ‘z’ or σ coordinates in the vertical; in this study we use the former. Although a finite difference model, it uses an unstructured coordinate system that introduces numerous computational efficiencies (Herzfeld, 2006). A suite of horizontal mixing, turbulence closure, advection schemes and open boundary conditions are available.

For the present simulations using the full hydrodynamic model, a k-ε turbulence closure scheme was used in the vertical, with Laplacian friction using the Smagorinsky parameterization in the horizontal. Lateral boundaries used a free-slip condition. The advection scheme for tracers was the ULTIMATE QUICKEST scheme (Leonard, 1991). Other details of the hydrodynamic model can be found in Herzfeld and Gillibrand (2015) and Schiller et al. (2015). The configuration of the model for each test case is described below.

3. Numerical Tests of the FFSL Scheme

The transport model has been tested in an idealised estuary, both closed and with an open boundary, and in a model of the Great Barrier Reef in Australia (the “GBR4” model). A selection of the test results are presented here. In both sets of tests, we have looked at four aspects of advection of a passive tracer:

(i) Does the transport model advection scheme produce comparable tracer distributions to those simulated by the full hydrodynamic model?
(ii) Is tracer mass conserved by the transport model?
(iii) Does the advection scheme meet constancy requirements i.e. does a domain-wide uniform tracer concentration of unity remain constant?
(iv) Is the scheme more computationally efficient?

For each test, the transport model was run three times using, in turn, the FFSL scheme, the traditional semi-Lagrangian advection scheme and the semi-Lagrangian with monotonic global filling. For the GBR4 test, we also ran a simulation using a semi-Lagrangian scheme with third order interpolation but no filling; this was designed to test the relative accuracy and speed of higher order semi-Lagrangian schemes relative to the FFSL method.
To illustrate the results of these tests, we present below images of tracer distributions from the full hydrodynamic model alongside comparable distributions from the transport model with the various advection schemes, and we derive estimates of errors between comparable results. The root-mean-square error (RMSE) between the hydrodynamic model prediction and transport model prediction over the length of each simulation was calculated at every wet grid cell, and maps of the RMSE are presented. We also present time series of tracer mass calculated by both models to illustrate mass conservation properties of the various schemes.

3.1 Closed Estuary

The first test was performed in an estuary basin closed to the sea. The basin had a depth of 20 m, shoaling along the estuary at the western side to 5 m depth at the head (Fig. 2). The eastern boundary was closed (effectively a wall). The horizontal grid spacing in both directions was 1000 m. In the vertical, 20 layers were used with a minimum thickness of 0.5 m in the upper 10 layers, increasing to a maximum of 5 m thickness. River flow into the estuary was 1000 m$^3$ s$^{-1}$, discharging at the head of the estuary. Since there is no ocean boundary, the estuary gradually filled up (steadily increasing sea level) due to the river inflow. No wind forcing was applied. Coriolis acceleration was imposed appropriate for latitude 38°S. With no wind stress or tidal forcing, the estuary was strongly stratified under the river plume.

Two passive tracer experiments were performed. In the first, the initial tracer concentration throughout the domain was zero and a point source of tracer was discharged in the centre of the basin (Fig. 2), at a rate of 1000 mg s$^{-1}$. Since there was no open boundary to the sea, no tracer should be lost from the model domain. A second tracer, with an initial concentration of 1.0 throughout the domain and a riverine concentration also of 1.0, was simulated to test constancy. Over the course of the simulation, concentrations of this second tracer should remain constant at exactly 1.0.

The simulations ran for 10 days. For this test, the hydrodynamic model ran with a 3D time step of 120 s and a 2D time step of 20 s. Output was stored at hourly intervals, with the transport model therefore running with a time step of 1 hour. Identical output of hourly concentrations of tracer throughout the model domain, were saved from both the hydrodynamic model run and the transport model runs for direct comparison.

After 10 days of simulations, a quasi-stable circulation had developed (Fig. 3). The seaward flow from the head of the estuary veered left (in the southern hemisphere) on entering the wider basin and was then steered along the closed eastern boundary, forming a cyclonic circulation in the estuary basin. A low-salinity plume was also steered around the perimeter of the estuary basin, leaving isolated pools of relatively high salinity in the central basin and in the south-west corner, where the circulation was weakest.
The tracer source was located within the north-eastward flowing branch of the circulation (Fig. 3). Consequently, released tracer was advected to the northeast in the full hydrodynamic model (HD), forming a distinct plume (Fig. 4a). After 10 days, tracer had been advected and diffused throughout most of the domain, with only the head of the estuary having tracer concentrations of zero (Fig. 4a). At the source location, concentrations were slightly less than 0.4 mg m$^{-3}$, but decreased rapidly with distance from the source. Concentrations throughout much of the basin were about 0.1 mg m$^{-3}$, but were closer to zero in the isolated central and south-western pools.

Simulated tracer distributions using the transport model with the FFSL algorithm exhibited qualitatively and quantitatively similar features to the full hydrodynamic model (Fig. 4b). After 10 days, the peak concentration at the source location was about 0.4 mg m$^{-3}$, very slightly higher than the HD case. Tracer concentrations through most of the basin were about 0.1 mg m$^{-3}$, with lower values in the isolated pools and at the head of the estuary. The main difference between the HD and FFSL schemes was a slightly increased tracer gradient immediately adjacent to the source location in the FFSL case: the grid cells to the east and northeast of the source in the HD model case had concentrations of 0.25 – 0.3, whereas in the FFSL case concentrations in those cells were 0.2 – 0.25 (cf. Fig. 4a and 4b). Outside the immediate source area, the FFSL results show good agreement with the HD model predictions.

Tracer distributions from the traditional semi-Lagrangian advection scheme and the semi-Lagrangian scheme with global filling are also presented in Fig. 4. Both semi-Lagrangian schemes produced the same general patterns of tracer distribution, but there are noticeable differences in the detail of the predicted concentrations from the full HD model. The semi-Lagrangian simulations produced a less diffuse plume of tracer away from the source, with consequently higher concentrations at the source location and along the initial plume trajectory. Further afield, tracer concentrations predicted by the traditional semi-Lagrangian scheme were generally lower throughout the estuary basin than those predicted by the HD model and FFSL scheme, partly due to mass loss (Fig. 4e) (see §3.4). In contrast, concentrations predicted by the semi-Lagrangian scheme with global filling were higher than the HD and FFSL distributions; the global filling adjustment tends to redistribute mass around the domain, thereby increasing the effective diffusion. It should be noted that a tri-linear interpolation scheme was used in the semi-Lagrangian model, effectively rendering the advection scheme to 1st order which is characterized by high numerical diffusion. In contrast, the Van Leer scheme used in FFSL is 2nd order accurate, and consequently far less diffusive.

The second tracer simulated remained constant throughout the simulation at exactly 1.0 mg m$^{-3}$, demonstrating that the key constancy condition was achieved.
3.2 Open Estuary

The second set of tests was performed in an identical estuary basin (Fig. 2), except that the eastern boundary was open. All conditions were as described above, with the addition of tidal forcing applied at the eastern boundary. The specified tide had an amplitude of 1 m and a period of 12 hours. River flow into the estuary was 1000 m$^3$ s$^{-1}$, discharged at the head of the estuary. No wind stress was applied.

The same two passive tracer experiments were performed as previously. The first tracer had an initial concentration of zero throughout the domain, with a point source of tracer discharging in the centre of the basin, at a rate of 1000 mg s$^{-1}$. At the open eastern boundary, a no-gradient condition was used during outflow and an oceanic tracer value of zero was specified during inflow. The second tracer had an initial concentration of 1.0 throughout the domain and riverine and open boundary concentrations also of 1.0, designed to test constancy.

The simulation ran for 10 days. As for the closed estuary test, the hydrodynamic model ran with a 3D time step of 120 s and a 2D step of 20 s, storing output at hourly intervals to force the transport model.

After 10 days simulation time, the mean circulation had reached a quasi-stable state (Fig. 5). As in the closed estuary, the seaward flow from the head of the estuary veered left on entering the wider basin, but in this case the outflow exited the estuary at the northern end of the open eastern boundary. The resulting cyclonic circulation in the estuary basin was therefore not closed, and the mean circulation in the south-eastern corner was very weak. The low-salinity plume exiting the estuary was also steered around the northern perimeter of the estuary basin, leaving a pool of relatively high salinity in the south-west corner.

Time series of modelled surface tracer concentrations at four point locations (Fig. 5) show largely good agreement between the HD model and the FFSL scheme (Fig. 6). Close to the source (Fig. 6a), the FFSL scheme reproduces the tidally-induced oscillations in concentration, though producing slightly lower values in the troughs than the HD model. During the latter half of the simulation, as a relatively steady state is reached, the agreement is very good. Further from the source, the relative errors increase somewhat, although the lower concentrations mean that the absolute errors decrease. However, the FFSL scheme clearly reproduced the timing of the tracer advection from the source location, and the evolution of concentration at each position.

The map of RMSE for the FFSL scheme confirms the decrease in absolute error with increasing distance from the source (Fig. 7). The RMSE had a maximum value of 0.26 at the tracer source and the error dropped rapidly away from the source. In contrast, RMSE values for both semi-Lagrangian schemes, with and without global filling, had peak values in excess of 0.4. Since the estuary is open, tracer was lost from the model domain when the plume reached the open eastern boundary. The south-east quadrant of the domain remained almost entirely free of tracer.
As in the previous test, the distribution obtained using the semi-Lagrangian advection scheme (with a monotonic global fill and open boundary adjustment) was more diffusive and errors were slightly larger throughout the domain away from the tracer plume. Although not shown here, the traditional semi-Lagrangian scheme without filling produced noticeably lower concentrations due to a consistent loss of mass (see §3.4).

Profiles of tracer concentration at four locations at the end of the 10-day simulation (Fig. 8) demonstrate that the FFSL scheme largely reproduced the vertical profiles predicted by the HD model in the stratified estuary. At the source location (Fig. 8a), agreement between the predicted profiles from the FFSL scheme and HD model was very good. The FFSL captured the sub-surface peak in concentration and the lower concentrations below 5 m depth. At increasing distance from the source (Fig. 8b-d), the FFSL model reproduced the changing vertical profile as tidal mixing eroded the vertical stratification. Some discrepancy in the absolute concentrations is evident, but the FFSL scheme captured the evolution of the tracer plume and declining concentrations with increasing distance from the source.

Constancy was also demonstrated in this test, with the second tracer remaining constant throughout the domain at exactly 1.0 mg m\(^{-3}\).

3.3 Great Barrier Reef Model

The realistic case chosen to assess the advection algorithm is that of the Great Barrier Reef (GBR) developed through the eReefs initiative (Schiller et al., 2014). The hydrodynamic component of this initiative represents the first time that a three-dimensional model has been applied to the whole reef, from Papua New Guinea to the south Queensland border (Fig. 9). Two models have been developed; a 4 km resolution model nested within the (non-tidal) OFAM 10 km resolution global model (Oke et al., 2008). This global model is based on MOM4p1 (Griffies, 2009) and delivers daily-mean outputs of sea level, T/S and 3D velocity at 10 km resolution around Australia. The low frequency sea level for the 4 km regional model was specified as the daily mean sea level from the global model, and this was superimposed with tidal heights from the global tide model of Cartwright and Ray (1990) using the implementation of Eanes and Bettadpur (1995). A 1 km resolution model is then nested within this 4 km model using output from the 4 km model on its boundaries. Both models use the Australian Bureau of Meteorology’s operational atmospherics models (ACCESS-A) for surface flux forcing at resolution of 12 km. The OFAM global model uses 3-hourly average surface forcing from the BoM’s operational global numerical weather prediction system (Seaman et al, 1995) and contains no tide.

The 4 km model (GBR4) has 48 vertical layers; at the surface the grid spacing is 1 m, extending from 2 m above mean sea level to 2 m below. Vertical grid spacing increases with depth to 200m at the deepest location (4000 m). The model allows wetting and drying, so that tidal flats
and shallow reefs are exposed at low tide (maximum tidal range is ~8 m in Broad Sound, central
GBR). The horizontal grid is also orthogonal curvilinear, so that there is local deviation in
horizontal resolution throughout the domain with a maximum grid spacing of ~6.6 km at the coast
at 19°S and minimum of ~3.2 km at 21°S. Gridlines are also not straight, but follow an S shape over
the north-south extent of the model. The heat flux was computed from standard meteorological
variables provided by ACCESS-A (wet and dry bulb temperature, air pressure, wind speed and
cloud amount) using short and longwave calculations outlined in Zillman (1972) and the bulk
method for sensible and latent heat using bulk coefficients of Large and Pond (1981). For the
surface freshwater fluxes, precipitation was provided by ACCESS-A and evaporation was
computed from the latent heat flux. Wind speed was converted to stress using the bulk scheme of
Large and Pond (1981). The model is forced with 22 freshwater inputs corresponding to the
discharge of the major river systems. These inputs were treated as Dirichlet open boundary
conditions with an imposed parabolic velocity profile whose vertical integral was equal to the
prescribed flow. The 3D time step is 90 s and the 2D step is 5 s. The GBR4 model has been run for
the period September 2010 – January 2015; for the tests described here, the model was hot-started
from the archive on 01 January 2011 and run for 30 days to 31 January 2011.

Tests were conducted using three distinct tracers, with differing initial concentrations and
source mechanisms. The time-step used for all transport model simulations was 1 hour, i.e. 40
times longer than the hydrodynamic time-step. The first tracer (passive tracer 0) was initialised
with concentrations of 1.0 and flushed via river discharge: all 22 rivers had a specified tracer
concentration of zero. Tracer concentrations at the open boundaries were specified as 1.0. The
second tracer (passive tracer 1) was initialised with concentrations of zero and supplied via four
discrete point sources in the domain (Fig. 9), with a source rate of 1000 mg s⁻¹. Open boundary
concentrations were zero. The third tracer (passive tracer 2) was designed to test constancy: initial
concentrations were set to 1.0, no point sources were implemented, and river and open boundary
concentrations were also set to 1.0. Modelled surface tracer distributions at the end of the month
long simulation, from both the hydrodynamic and transport models are shown below.

The surface concentrations of passive tracer 0, resulting from the input of river water with
tracer concentrations of zero, are shown for the central GBR (Fig. 10) and around the Fitzroy River
in the southern GBR (Fig. 11). In the hydrodynamic model results, the riverine water produced a
zone of reduced tracer concentration close to the shore, with mixing between the ambient GBR
water and the intruding boundary water leading to zones of intermediate tracer concentrations.
Outside the nearshore zone, water properties were not modified by the river inputs and the tracer
concentration remained steady at 1.0. The distributions of passive tracer 0 from the FFSL
advection scheme closely matched that from the full hydrodynamic model in terms of spatial extent
of the river plumes and concentrations therein, with RMSE values (calculated over the full
simulation) less than 0.2 and, over most of the domain less than 0.1 (Fig. 10b). The traditional
semi-Lagrangian scheme was far more diffuse, with tracer spreading offshore to more than twice
the extent as the hydrodynamic model. RMSE values of, or exceeding, 0.2 extended over much
wider areas of the model domain (Fig 10c). The FFSL scheme again provided a better, less
diffusive, representation of the HD model advection than the semi-Lagrangian scheme in this test.
The concentrations of tracer predicted by the various schemes in the Fitzroy Estuary region
confirm the better performance of the FFSL scheme (Fig. 11). Using a third order interpolation
with the semi-Lagrangian method improved the accuracy of the scheme, but still produced inferior
results compared to the FFSL scheme.

The plumes of the second tracer (passive tracer 1) after 30 days simulation time are shown in
Figs. 12 and 13. The semi-Lagrangian distributions were again more diffuse, resulting in lower
concentrations at the source and exhibiting less defined frontal structure, producing much larger
errors (Fig 12). In contrast, the less diffuse hydrodynamic and FFSL distributions resulted in larger
maximum concentrations at the source (e.g. for the northernmost source, peak concentrations at the
end of the simulation were 0.047, 0.036 and 0.027 mg m\(^{-3}\) for HD, FFSL and semi-Lagrangian
respectively) and produced more defined frontal boundaries and plume structure, with much
reduced error values. The FFSL distributions compared very favourably with the hydrodynamic
solutions. In this case, although inferior to the FFSL scheme, the semi-Lagrangian scheme also
produced acceptable spatial plume distributions. The simulation performed was not long enough
for tracer to reach the open boundary, whereas in simulations where tracer is imported or exported
from the domain, the global filling adjustment may lead to the semi-Lagrangian scheme producing
more diffusive distributions.

No introduced maxima or minima were evident in the FFSL distribution for passive tracer 2,
with concentrations remaining constant at exactly 1.0 throughout the domain, indicating that the
constancy condition was satisfied. Semi-Lagrangian schemes should also always satisfy
constancy, because the material derivative is used to update concentrations.

Overall, the FFSL scheme out-performed the semi-Lagrangian schemes on the basis of
distribution of tracer compared to the hydrodynamic baseline. The conservation of mass achieved
by all the schemes and the relative computational speeds are considered in the next sections.

3.4 Mass Conservation

Total mass conservation was good for all schemes except the traditional semi-Lagrangian
advection (Fig. 4e). In the closed estuary test case, when all discharged mass should remain within
the system, the HD model and both the FFSL and semi-Lagrangian with monotonic fill schemes
conserved more than 99% of the discharged tracer over the 10 day simulation. In contrast, without
the global fill correction, the traditional semi-Lagrangian scheme began to steadily lose mass after
4 days, and the total mass remained relatively steady with only about 50% of the discharged tracer mass accounted for.

In the open estuary test case, mass was lost through the open boundary (Fig. 7e). But the rate of loss was very similar in the HD, FFSL and semi-Lagrangian with global fill simulations. In contrast, the traditional semi-Lagrangian scheme lost mass at a much greater rate, as the loss through the open boundary was compounded by a numerical loss of mass due to the scheme itself; the calculated mass lost does not therefore accurately reflect the real loss through the open boundary.

For the GBR simulations, the FFSL and globally filled semi-Lagrangian scheme conserved mass with little error, whereas the traditional semi-Lagrangian scheme introduced deviations in total mass throughout the simulation, with an oscillation in total mass at the tidal frequency (Fig. 14). This simulation was too short to allow tracer to reach the open boundaries, so no mass was lost from the model domain; in a longer simulation, it is anticipated that errors in the estimation of open boundary mass fluxes would also have resulted in a deterioration of mass conservation in the globally filled semi-Lagrangian method.

3.5 Comparative Model Speeds

The results shown previously have illustrated the accuracy and conservation properties of the FFSL advection scheme. A further requirement of a transport model is that it runs efficiently; the proposed scheme will be used to simulate advection in sediment transport and biogeochemical models, within which numerous tracers must be advected. The semi-Lagrangian transport model is typically an order of magnitude faster than the full hydrodynamic model when run with a small number of tracers and a longer time step, as in these test cases. The FFSL scheme needs to be of comparable efficiency, and to scale up efficiently from few to many tracers.

The model speeds for the test runs described above are presented in Table 1. The model speed is defined as the length of the simulation divided by the wall time of the run; e.g. a runtime of 100:1 will complete 100 model days in 1 actual day. So, if a model simulation of one month (30 days) takes one day to complete, the model speed is given as 30. The model speed is also machine-dependent, and the speed of the full hydrodynamic (HD) model is also dependent on the number of processors (cores) used. In all the tests, the transport model was run on the same machine as the equivalent HD model simulation but used only one core. The number of cores used in the HD model simulation is shown in the table. The table shows that for these simulations, with typically 2 – 3 tracers, the FFSL is comparable or quicker than the various semi-Lagrangian schemes. Both schemes are over an order of magnitude faster than the hydrodynamic model. This result clearly illustrates the value of the transport model, since this speedup is considerable and allows vastly more modelling throughput. The speedup is also domain-dependent, and in our experience it is not
unusual to achieve up to three orders of magnitude speedup on some domains, compute infrastructure and tracer configurations. The semi-Lagrangian scheme is slowed by the necessity to implement the global filling and open boundary adjustments to ensure global mass conservation.

The challenge remaining to the FFSL scheme is to determine how well it scales up to large numbers of tracers. In the experiments undertaken so far, we have found that the fully 3D COSMIC scheme is about 15% slower than the quasi-3D FFSL scheme. A biogeochemical model of the GBR region utilizing 60 advected / diffused biogeochemical and sediment tracers appears to be about only 10% slower using FFSL than the semi-Lagrangian advection scheme. This is due to the more efficient scaling with the semi-Lagrangian scheme as the number of tracers increases, but nevertheless indicates that the FFSL scheme is viable for use with large biogeochemical models. Work currently underway to implement the FFSL algorithm using multi-threading should also improve computational performance.

4. Discussion and Conclusions

The flux-form semi-Lagrangian scheme presented in this paper offers a potential solution to the problem of running coastal biogeochemical and sediment transport models offline, where fast run times and conservation of tracer mass are prerequisites. By applying semi-Lagrangian methods to the volume fluxes across cell faces, following the methods of LR96 and Leonard et al. (1996), rather than to the cell-centred tracer distribution itself like traditional semi-Lagrangian advection schemes, the FFSL scheme provides an accurate, efficient and mass-conservative transport model for application on curvilinear grids typical of coastal ocean models. Our results from both the test estuary cases and the GBR domain demonstrate that the offline transport model produces tracer distributions that are comparable with those produced by the hydrodynamic model itself. Some differences between the resulting distributions are inevitable: the transport model, in our examples, uses hourly-mean velocity and volume flux data, whereas the hydrodynamic model has time steps of typically 1 – 2 minutes; the resultant smoothing of the velocity and flux fields eliminates some of the variability in the advection of tracer simulated by the hydrodynamic model. However, the objective of the study is to achieve savings in computational time, and some sacrifice in the accuracy of the results must be expected. The key benefits of the FFSL advection scheme are that it produces comparable results to the original hydrodynamic model at a much lower computational cost, allowing greater simulation capacity and scenario testing.

Although the FFSL scheme allows long time steps relative to the Courant number, the scheme is not, unlike the semi-Lagrangian method, unconditionally stable. The Lipschitz condition, expressed by Equations 15 and 16, is relatively mild compared to the Courant-Friedrichs-Lewy (CFL) condition; nevertheless, we found the FFSL scheme to be sensitive to the condition, and found it necessary to build checks into the model code to prevent instabilities developing: if the
Lipschitz limit is approached, the model is forced to temporarily use a smaller sub-time-steps until the Lipschitz condition is satisfied again by the full time step. The Lipschitz condition essentially prevents backwards trajectories from overlapping, which would destabilize the mass balance calculation. It is important to remember that whilst the traditional semi-Lagrangian scheme is unconditionally stable, it does not necessarily follow that it is accurate when large time steps are used. Our results suggest that semi-Lagrangian schemes lack the accuracy and mass conservation of the FFSL scheme; even with *a posteriori* global filling (Rood, 1997; Priestly, 1993) accuracy is diminished, as the mass restoration acts as a diffusive influence on tracer distributions. However, the accuracy of the FFSL scheme is also sensitive to the time step used; as the time step increases, the backwards trajectory will lengthen, and on a curvilinear grid a longer trajectory potentially becomes increasingly inaccurate. Some experimentation to find a time step appropriate for each numerical grid will be necessary.

That the FFSL scheme is able to use long times steps is due to the stabilizing influence of the transverse terms $f(\theta)$ and $g(\theta)$ in Equation 4 (LR96; Leonard et al., 1996). The transverse terms are computed using the advective form of the conservation equation, and the flux form is subsequently applied to these transverse terms, thus ensuring conservation. The Van Leer scheme was used to compute the tracer value at the face in the fractional component of Equation 10; in practise, however, any advection scheme may be used. LR96 applied the transverse terms only to the horizontal flux terms, assuming that the vertical motion is essentially independent, whereas Leonard et al. (1996) applied the transverse terms in all three dimensions. The latter approach leads to greater computational cost but increased numerical stability. In the test cases presented here, we found little difference between the results obtained using the two approaches, but the simulations using the LR96 approach were noticeably quicker, by up to about 15%. It seems likely that in many oceanographic applications the quasi-3D scheme of LR96 will be sufficiently stable to make the computational cost savings worthwhile; but it is also likely that for some environments, the full 3D application of Leonard et al. (1996) will be necessary to retain numerical stability. To ensure numerical stability, Leonard et al. (1996) found it necessary to use upstream cell face velocities, rather than cell-centred velocities, to calculate the transverse terms; we also, after some experimentation, adopted that approach.

Our tests only used two or three tracers. Traditional semi-Lagrangian advections schemes (e.g. Staniforth and Cote, 1991) are efficient for models using many tracers because much of the computational effort is spent calculating the back-trajectory, which only needs to be calculated once; the same trajectory applies to all tracers. The same approach can be taken for the FFSL scheme, with the back-trajectories for every cell face and cell-centred velocity calculated just once and used for the local mass balance calculation for every tracer. For two and three tracers, this approach results in a computational efficiency comparable to the traditional semi-Lagrangian approach; preliminary results using a full biogeochemical model indicate that FFSL is only
marginally slower than the semi-Lagrangian scheme. There seems little reason that efficiency of
the FFSL scheme should deteriorate relative to semi-Lagrangian schemes, particularly since the
semi-Lagrangian scheme requires the additional step of global filling to ensure mass conservation,
which the FFSL scheme does not need.

We have presented results from some relatively short simulations. Longer runs, on seasonal or
annual time scales, using offline transport models often present storage problems, requiring large
volumes of 3D velocity, volume flux, vertical mixing and scalar results from the parent
hydrodynamic model to be archived. Accessing such large files may potentially reduce model
efficiency and make long runs unviable. Data from the GBR4 hydrodynamic model described here
are stored in multiple files each containing a calendar month of data. Using these data with the
FFSL scheme, Schiller et al. (2015) ran a tracer simulation of 3.5 years duration with good
transport model performance characteristics. With careful data management then, the FFSL
scheme appears to be a viable option for long (multi-year) scalar transport simulations. It should be
noted that this ability to perform long runs with the present model is made possible partly by the
sparse coordinate system of the hydrodynamic model (Herzfeld, 2006), which stores only the
variable values from wet grid cells, significantly reducing the file size.

In conclusion, the FFSL scheme presented here provides an accurate and mass-conserving
advection scheme that may be used to simulate the transport of tracers in offline coastal ocean
models. The scheme is comparable in terms of computational efficiency to traditional semi-
Lagrangian advection schemes, but offers more accurate solutions relative to the source
hydrodynamic model results. As such, the scheme should offer an opportunity for marine
biogeochemical, sediment transport and water quality modellers to move their models offline
without suffering from loss of mass or unacceptable inaccuracy as a consequence.

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helpful comments.
References


Table 1. Comparative model speeds of the full hydrodynamic model (HD) and the transport model with various advections schemes: the FFSL advection scheme, the traditional semi-Lagrangian scheme with no filling, traditional semi-Lagrangian scheme with global filling, and a semi-Lagrangian scheme using 3rd order interpolation with no filling. The comparison is very machine-dependent; in all tests, the transport model simulations were run on the same machine as the HD model, with the same number of passive tracers. The number of processors (cores) used by the HD model is shown; in all cases, the transport model used one core.

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Figure 1. Schematic illustrating the integer and fractional components of the semi-Lagrangian trajectory for the velocity component \( U \) on a curvilinear grid, where \( U \Delta t > 2h_i \). The cases of (a) a cell-centred velocity, \( U_i \), and (b) a face velocity \( U_{i+\frac{1}{2}} \), are illustrated. The dashed vertical lines indicate the lines of the cell centres (i, i-1, i-2); solid lines indicate the faces of each cell (i-\( \frac{1}{2} \), i-\( \frac{3}{2} \), i-\( \frac{5}{2} \)). The heavy dashed line indicates the trajectory bounded by the filled circles. In the cases shown, values of \( K \) are negative since \( U \) is positive.
Figure 2. Bathymetry of the test estuary basin. The closed estuary basin is shown. For the open basin, the mouth of the estuary from south to north is opened to the adjacent ocean with water depths of 20m. The location of the source of passive tracer is indicated by the white triangle.
Figure 3. Modelled surface salinity and current vectors after 10 days in a simulation of a closed estuary. Discharge at the head of the river was 1000 m$^3$ s$^{-1}$. Initial salinity was 34.
Figure 4. Passive tracer distributions after 10 days of discharge in a closed estuary, simulated by:
(a) the full hydrodynamic model, (b) the transport model with FFSL advection, (c) the transport model with a traditional semi-Lagrangian advection scheme, (d) the transport model with a semi-Lagrangian scheme plus global filling. (e) The total tracer masses in the model domain for each scheme over the integration period, together with the cumulative mass released.
Figure 5. (Left) Modelled surface salinity and current vectors after 10 days in a simulation of an open estuary. Discharge at the head of the river was 1000 m$^3$ s$^{-1}$, and the S$_2$ tidal amplitude was 1.0 m. The four closed circles (●) indicate the locations from where time series (Fig. 6) and vertical profiles (Fig. 8) of tracer were extracted; the southernmost point coincides with the tracer source. (Right) Profile of salinity at the tracer source location after 10 days simulation.
Figure 6. Time series of modelled surface tracer concentration from the HD model and FFSL scheme at the four point locations indicated in Fig. 5. Distance from the source increases from (a) – (d). RMSE values for each series are indicated.
Figure 7. (a) Passive tracer distributions after 10 days of discharge in an open estuary, simulated by the full hydrodynamic model; (b) RMS error for the transport model simulation with FFSL advection; (c) RMS error for the transport model simulation with a semi-Lagrangian advection scheme; (d) RMS error for the transport model with a semi-Lagrangian scheme plus global filling. The total tracer masses in the model domain over the integration, and the mass released, are shown in (e) for each scheme. Note the loss of tracer through the open mouth beginning after ~5 days.
Figure 8. Vertical profiles of tracer concentration after 10 days at four locations (Fig. 5) in the open estuary simulation. The profiles from the hydrodynamic model (HD model, bold lines) are contrasted with the profiles generated by the FFSL scheme in the transport model (FFSL, light lines). Distance from the source increases from (a) – (d).
Figure 9. Locations (▲) of the sources of passive tracer 1 in the Australian Great Barrier Reef (GBR4) model domain, overlain on the model bathymetry.
Figure 10. (a) Surface distributions of Passive Tracer 0 in the central GBR after 31 days simulation by the hydrodynamic model (HD); (b) RMS error for the transport model using the FFSL scheme relative to the HD model, calculated over the 31-day simulation; (c) RMS error for the transport model using the semi-Lagrangian advection scheme (no fill). The initial tracer distribution (C = 1.0) was being flushed by river discharges (C = 0.0).

Figure 11. Surface distributions of Passive Tracer 0 from the Fitzroy Estuary in the southern GBR after 31 days simulation: (a) hydrodynamic model; (b) FFSL scheme; (c) traditional semi-Lagrangian scheme (no filling); (d) third order semi-Lagrangian scheme (no filling). The initial tracer distribution (C = 1.0) was being flushed by river discharges (C = 0.0).
Figure 12. (a) Detailed surface distribution of the three southern-most releases of Passive Tracer 1 in the central GBR after 31 days simulation by the hydrodynamic model (HD); (b) RMS error for the transport model using the FFSL scheme relative to the HD model, calculated over the 31-day simulation; (c) RMS error for the transport model using the semi-Lagrangian advection scheme with global filling.

Figure 13. (a) Detailed surface distribution of the northern-most release of Passive Tracer 1 in the GBR after 31 days simulation by the hydrodynamic model; (b) RMS error for the transport model using the FFSL scheme relative to the HD model, calculated over the 31-day simulation; (c) RMS error for the transport model using the semi-Lagrangian advection scheme with global filling.
Figure 14. Total mass of Passive Tracer 1 after 31 days of simulation in the GBR, simulated by the transport model with FFSL (‘FFSL’), the transport model with a semi-Lagrangian scheme plus global fill (‘LAG FILL’), the transport model with a traditional semi-Lagrangian advection scheme (‘LAG NOFILL’) and the theoretical input of mass into the domain (‘THEORY’). Total mass is represented as the percentage of the final mass.