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A mass-conserving advection scheme for offline simulation of scalar transport in coastal ocean models

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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.

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 utilise 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 that 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 discretisation 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 discretised scalar advection equation reduces to the discretised 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 discretisation 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

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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, 2007). Additionally, Naifar et al. (2007) addressed consistency by computing new flow fields for the transport scheme.

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 discretised 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 apply 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, which allows long time steps (relative to the Courant restriction) for computational efficiency but which also conserves mass. In the following sections we describe the scheme, apply it to two idealised 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 φ conservatively with the ability to use long ($C_r \gg 1$) time steps, where $C_r = \max(u_1\Delta t/h_1,\ u_2\Delta t/h_2,\ w\Delta t/h_3)$ is the Courant number. From the prior hydrodynamic model simulation, the cell dimensions (h_1, h_2, h_3), instantaneous sea surface elevation $\eta^n_{i,j}$, time-averaged volume fluxes $(u_1h_2h_3)^{n+1/2}_{i\pm1/2,j}$ and $(u_2h_1h_3)^{n+1/2}_{i\pm1/2,j}$, 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:

$$\frac{\partial \eta}{\partial t} + \nabla_H . \int_{-H}^{\eta} \vec{u} \cdot dz = 0 \qquad (1)$$

where $\vec{u}$ is the three-dimensional velocity vector, ∇_H is the horizontal divergence operator and z is the vertical coordinate. Satisfying Eq. (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

$$\Delta\eta = \int_{t_1}^{t_2} \eta dt \neq \nabla_H D \int_{t_1}^{t_2} \vec{U} dt$$