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A new approach to the local time stepping problem for scalar transport

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ABSTRACT

A new scalar transport method is proposed to reduce computational time when a large number of scalars are transported in coupled hydrodynamic-ecosystem models. The new Local Mass Transport (LMT) method confines subtime transport computations to regions where the local Courant–Freidrichs–Lewy (CFL) number exceeds a given numerical stability criteria for a global (large) time step, but the method does not require either contiguous regions or special boundary algorithms between regions as used in previous Local Time Stepping (LTS) approaches. The new method uses conservative transport of mass rather than dissolved concentration. This approach allows different faces of a single grid cell to use different subtime steps. The new LMT method is further extended to include background filtering (LMTB) so that scalars below a pre-defined background concentration are ignored in transport calculations. This new approach can further reduce computational time where large regions are at or below an irrelevant background concentration. Both LMT and LMTB methods can be more computationally efficient than global subtime stepping.

1. Introduction

1.1. Transporting mass instead of concentration

The transport of scalars in hydrodynamic modelling is conventionally based on transport of dissolved concentrations. The standard 3D advection–diffusion equation uses volume concentration of a dissolved constituent, c, typically written as

$$\frac{\partial c}{\partial t} = -\frac{\partial}{\partial x_j}(u_j c) + \kappa \frac{\partial^2 c}{\partial x_j \partial x_j} + s_{net} \tag{1}$$

where u_j is the velocity field, κ the diffusivity, s_{net} a net source/sink, and the Einstein summation convention is used for repeated subscripts. In a control-volume formulation, this is commonly written as

$$\frac{\partial}{\partial t}\int_V c dV = -\int_S (u_j c)\hat{n}_j dS + \int_S \kappa \frac{\partial c}{\partial x_j}\hat{n}_j dS + \int_V s_{net} dV \tag{2}$$

where V is a control volume and S is the area of the surrounding control surface and $\hat{n}_j$ is a unit vector normal to the surface. Numerical time-marching for the concentration from time step n to $n+1$ at cell location (i) can be represented as

$$c_i^{n+1} = c_i^n + \Delta t f(c, \kappa, u, a, s_{net}) \tag{3}$$

where subscripts indicate discrete cell location, superscripts indicate time level, Δt is the time step, and $f()$ is a discrete function representing the *spatially-averaged* effects of neighbor values for the independent variables. For a system that allows temporally-changing control volumes, an equivalent conservative function is

$$c_i^{n+1} = \frac{V_i^n}{V_i^{n+1}} c_i^n + \frac{\Delta t}{V_i^{n+1}} g(c, \kappa, u, a, s_{net}) \tag{4}$$

where $g()$ is a discrete function representing the *integrated* effects of neighbor values for the independent variables, and $V_i^{n+1} \neq V_i^n$ typically occurs for a moving free surface within a fixed 2D or 3D grid.

A slightly different approach can be developed by considering the transport of scalar mass, m as

$$\frac{\partial m}{\partial t} = \frac{\partial}{\partial t}\int_V c dV \tag{5}$$

The left-hand-side of Eq. (2) can be replaced with $\partial m/\partial t$ and the right-hand-side interpreted as the rate of change of mass in a control volume; it follows that Eq. (4) can be replaced with

$$m_i^{n+1} = m_i^n + \Delta t g(c, \kappa, u, s_{net}) \tag{6}$$

which can be recognized as Eq. (4) multiplied through by V_i^{n+1} using $m = cV$; thus a change from transporting concentration to transporting mass might be a relatively trivial alteration to many numerical models. However, to close a mass transport equation set for known u, κ, and s_{net}, two additional equations are required. First,

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the conservation of volume for an incompressible fluid, which can be written as

$$\frac{\partial V}{\partial t} = -\int_S u_j \hat{n}_j \, dA \tag{7}$$

where subscripts are vector indexes using the Einstein summation convention and volume sources/sinks are neglected. Second, we require a diagnostic definition of concentration, mass, and volume relationships:

$$c = \frac{m}{V} \tag{8}$$

which can be applied discretely at any time level n and grid cell i.

The above observations might seem trivial; indeed, the volume change is typically computed in hydrodynamic simulations with a free surface, and no doubt many models actually compute m as a step in computing c. Nevertheless, as illustrated herein, this minor change in viewpoint – from transporting concentration to transporting mass – provides interesting new possibilities for numerical algorithms that have not previously been exploited.

1.2. Motivation

A difficulty for coupled hydrodynamic, pollutant (e.g. oil spill) and water quality/ecosystem models is the computational expense of transporting scalars. In particular, ecosystem models often represent multiple species of phytoplankton, zooplankton and speciation of nutrients, e.g. nitrate, ammonium, organic nitrogen, phosphate, and organic phosphorous (e.g. Camacho and Martin, 2013; Leon et al., 2012; Marinov et al., 2008; Robson and Hamilton, 2004). Even in strictly hydrodynamic models, a large number of transported tracers can be effective in visualizing and quantifying circulation or possible pollutant behavior, thus adding to computational costs (e.g. Young et al., 2011). Indeed, herein the transport of 41 scalars in a hydrodynamic model results in the scalar transport computational time ranging from 15 to 30 times greater than the hydrodynamic computational time when using conventional transport methods (see Section 3.3).

Such computational costs can be exacerbated by localized regions where the Courant–Friedrichs–Lewy (CFL) number (CFL = $u\Delta t/\Delta x$) at a desired large time step exceeds a numerical stability constraint. In general, a large model time step is incompatible with large velocities relative to the space discretization (with the constraint quantitatively depending on the numerical method used for scalar transport), so the allowable transport time step must be controlled to limit the CFL everywhere in the domain. A high velocity in a single grid cell can require a reduced time step for the entire domain and thus increase model computational time. This constraint becomes even more problematic when unstructured or curvilinear grid system are used with a large range of cell sizes (Dawson et al., 2013).

Further contributing to transport costs is an apparently unrecognized problem: the expense of transporting zero concentrations for phenomena that are strictly confined to a local area (e.g. an oil spill). A similar problem arises in transport of water quality constituents below a background concentration that does not affect the ecosystem behavior. For example, if a nutrient along a coastal shelf has some background level that is invariant outside of a river plume, why bother transporting the nutrient outside of plume waters? When a pollutant has been diffused below detection limits and below any ecosystem concern, why continue to track irrelevant and unconfirmable concentrations? It seems likely that extensive computational time in ecosystem and pollutant models is expended simply shuffling around irrelevant changes in background or zero concentrations.

In this paper, methods for Local Mass Transport (LMT) and Local Mass Transport with Background filter (LMTB) are proposed as new ways to address these issues. These algorithms are radical departures from previous scalar transport methods and provide an opportunity to rethink the way we compute scalar fields.

1.3. Background

There is a performance mismatch between most hydrodynamic and scalar transport models for localized high velocity conditions when using finite difference/volume methods. Many hydrodynamic models only retain their theoretical accuracy order for CFL $< O(1)$, where the exact CFL limit for accuracy depends on the discretization scheme (Hodges, 2004). However, it has long been understood that implicit and semi-implicit hydrodynamic models are both stable and reasonably accurate for $1 <$ CFL < 5, especially when high CFL numbers are locally confined in space and/or time. Modelers concerned about computational costs take advantage of this robustness by setting the largest possible hydrodynamic time step such that CFL < 1 is achieved over most of the domain, but increased error is accepted in localized regions where CFL > 1. Momentum conservation can remain stable and reasonably accurate with locally-high CFL numbers simply because momentum equations are globally biased towards losses (i.e. dissipation). Unfortunately, common Eulerian conservative scalar transport methods are not as robust when locally-high CFL numbers are encountered. Conservative scalar transport at high CFL typically results in unrealistic local concentrations that rapidly degrade simulation accuracy. The fundamental difficulty for scalar transport with high CFL is the increasing number of neighbor cells influencing the concentration in a single grid cell over a model time step, i.e. the "domain of dependence" illustrated in Fig. 1. These issues are well understood and are often addressed by use of semi-Lagrangian schemes (e.g. Blossey and Durran, 2008; Lentine et al., 2011; Manson and Wallis, 2000) that track back along hydrodynamic characteristics to ensure the correct domain of dependence is achieved. Leonard (2002) showed that these ideas could be used to define unconditionally stable Eulerian and semi-Lagrangian schemes for high CFL numbers based on the discrete stencil "sweep point" and "balance point." Despite these advances, many coupled hydrodynamic-water quality models still rely on simple transport schemes where selection of a sufficiently small model time step is required to prevent locally-high CFL numbers that exceed the CFL stability constraint.

Parallel to development of the finite-difference methods described above, approaches for handling locally-high CFL numbers in finite element models have been constructed following the ideas of Osher and Sanders (1983), which are now known as Local Time Stepping (LTS) algorithms. These methods have a rich finite element literature, where the effects of locally-refined unstructured grids have made their use almost a necessity (Constantinescu and Sandu, 2007; Coquel et al., 2010; Crossley and Wright, 2005; Dawson and Kirby, 2001; Krivodonova, 2010; Sanders, 2008; Seny et al., 2013; Tang and Warnecke, 2006; Zhang et al., 1994). These methods typically involve separating a domain into regions sharing similar CFL constraints such that small time steps are used only where locally necessary. LTS requires identifying and treating the interface between regions with specialized algorithms to handle the change in time step, so the number of regions affects the efficiency of the system. Much as domain decomposition methods are used for separating a large computational space into separate subregions with different grid resolution, LTS can be considered an approach to time decomposition (Shishkin and Vabishchevich, 2000). The LTS idea has also been extended to multiscale modelling (Muller and Stiriba, 2007; Schlegel et al., 2012). A similar regionalization approach is also found in the finite-difference literature