Author's response to discussion of *Derivation of high-order advection-diffusion schemes* by Pavel Tkalich, 2006 *J. Hydroinf*. 8(3), 149–164

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The Author would like to thank the Discusser (Cunge 2007) for critical reading of paper published by Tkalich (2006). The discussion is focused on derivation of numerical methods for the model advection equation

$$\frac{\partial \phi}{\partial t} + u\frac{\partial \phi}{\partial x} = 0, \tag{1}$$

where $\phi(t, x)$ is a advected scalar (such as concentration of admixture in water bodies); u is the advecting velocity; x is the spatial coordinate; t is the time. In the original advection-diffusion equation the velocity is assumed to be uniform and positive, and the diffusion term is ignored as unimportant to the topic of discussion.

One of the purposes of the research paper (Tkalich 2006) was to offer a uniform procedure to derive a suit of effective and accurate explicit numerical methods for the solution of equation (1). An intimate connection between different well-known schemes, such as first-order upwind, Lax-Wendroff (Lax & Wendroff 1960, 1964), and QUICK-EST (Leonard 1979), is demonstrated using Lagrange polynomials, although one might use Hermite polynomials or other techniques to obtain similar results. One may agree that there is no absolute best procedure for numerical schemes derivation, as well as there is no absolute best all-purpose numerical scheme. After becoming acquainted with pioneering work by Holly & Preissmann (1977) years ago, the excellent method was the first choice of the Author due to the same arguments as presented by the Discusser. However, at the later stage the Author became involved with other types of schemes due to several issues outlined below. The discussion extends beyond merely a comparison of two (types of) schemes to move a little further toward advocating some new trends emerging in computational methods. Due to the limited scope of the dialog, the paper is by no means a complete review.

doi: 10.2166/hydro.2007.002

MASS CONSERVANCY

The modern trend is to use schemes which could be expressed in the conservative form

$$\phi_i^{k+1} = \phi_i^k - \alpha((\phi_E)_i - (\phi_W)_i), \tag{2}$$

where ϕ_i^k is the cell-averaged value of the transported scalar ϕ at the i-th computational cell at time-level k; $(\phi_W)_i$ and $(\phi_E)_i$ are the west- and east-face values of the transported scalar for i-th computational cell (shaded in Figure 1); $\alpha = u\Delta t/\Delta x$ is Courant number; Δx is the grid size; Δt is the time-step. Conservative form (2) is important because mass conservation is guaranteed if ϕ_W for the cell i equals ϕ_E for the neighbor cell (i-1), or $(\phi_W)_i = (\phi_E)_{i-1}$; naturally $(\phi_W)_{i+1} = (\phi_E)_i$. Unfortunately this property was often ignored in many earlier algorithms.

COMPACTNESS

The face values represent integrated over Δx and Δt values of the transported scalar ϕ at the west and east boundaries

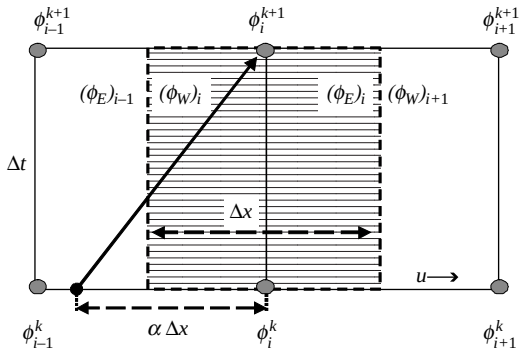

Figure 1 | Computational grid.

of a computational cell. It is a convenient quantity to rewrite high-order schemes utilizing extensive computational stencils in the short form (2). In fact, this is a two-step algorithm, where the first step is to compute face values using one of the formulae given in Appendix A of the discussed paper, and the second step is to apply expression (2) for each computational cell using two face values associated with the cell. If one rewrites (2) in a single-step updated form by explicitly substituting expressions for face values, the update reveals real stencil used by the scheme; i.e. even though the formulation (2) looks like a compact, it might use more than two (nodal) values. For instance, east-face value $(\phi_E)_i$ for QUICKEST (3UP) algorithm is using a 3-node stencil $\left\{\phi_{i-1}^k, \phi_i^k, \phi_{i+1}^k\right\}$, but a single-step update is based on 4 nodes $\left\{\phi_{i-2}^k, \phi_{i-1}^k, \phi_i^k, \phi_{i+1}^k\right\}$.

Similarly, the Holly-Preissmann method is a two-step algorithm, where at the first step derivatives $(\phi_x)_i^*$ are computed for each node utilizing four-component stencil $\left\{\phi_{i-1}^k, \phi_i^k, (\phi_x)_{i-1}^k, (\phi_x)_i^k\right\}$, and the second step provides sought values ϕ_i^{k+1} at similar stencil $\left\{\phi_{i-1}^k, \phi_i^k, (\phi_x)_{i-1}^*, (\phi_x)_i^*\right\}$. A single-step update obtained by combining the two steps reveals that the stencil of the Holly-Preissmann method is stretched over 3 nodes (or two space intervals) as $\left\{\phi_{i-2}^k, \phi_{i-1}^k, \phi_i^k, (\phi_x)_{i-2}^k, (\phi_x)_{i-1}^k, (\phi_x)_i^k\right\}$. Strictly speaking, based on a single-step update form, none of the two schemes discussed above could be qualified as compact, and both methods are equally "compact" at the final stage alone.

Since the computational science has moved toward high-order algorithms, one has to accept the involvement of more than two components in a computational stencil, either in terms of spatial or temporal extensions, or via the introduction of new variables. The assessment of efficiency of an algorithm could be a problem-depended, and by no means a straightforward procedure.

BOUNDARY AND OTHER AUXILIARY CONDITIONS

During the era dominated by first-order schemes, boundary conditions were treated using value of the transported scalar at imaginary node ϕ_{i-1}^k (for the situation shown in Figure 2). The Dirichlet boundary condition ($\phi = f_B$) for the first-order upwind scheme (1UP) could be satisfied assuming $\phi_{i-1}^k = f_B$ or simply $\phi_i^{k+1} = f_B$. The Neumann boundary condition ($\partial\phi/\partial x = 0$) could be prescribed as $\phi_{i-1}^k = \phi_i^k$. Incidentally, face values for the first-order upwind scheme coincide with the nodal values, i.e. $(\phi_W)_i = \phi_{i-1}^k$ and $(\phi_E)_i = \phi_i^k$. After the introduction of high-order methods, similar attempts have still been occasionally practiced to satisfy auxiliary conditions in terms of nodal values, leading to unnecessary complexity of an overall algorithm and error accumulation at areas of discontinuity. The conservative form (2) offers an easy and accurate alternative to prescribe discontinuities in terms of face values $(\phi_W)_i$, $(\phi_E)_i$ or fluxes $\alpha(\phi_W)_i$, $\alpha(\phi_E)_i$. For all schemes mentioned in the paper (Tkalich 2006) the Dirichlet condition is satisfied when $(\phi_W)_i = f_B$, and the Neumann condition is simply $(\phi_W)_i = (\phi_E)_i$. Additionally one can use the cell averaged value ϕ_i^k to prescribe more complex cases.

MULTI-DIMENSION EXTENSION

It should be noted that the majority of schemes considered in the discussed paper have been (or could be) extended to

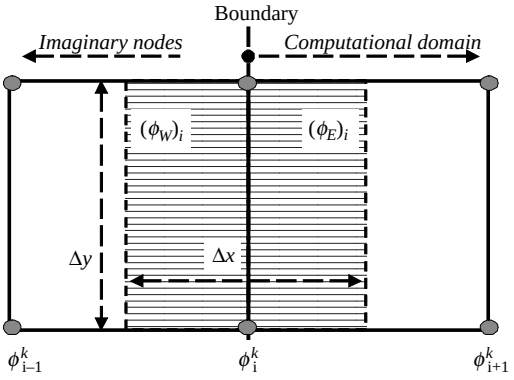

Figure 2 | Sketch of computational grid near boundary.

two dimensions (2-D)

$$\frac{\partial \phi}{\partial t} + u\frac{\partial \phi}{\partial x} + v\frac{\partial \phi}{\partial y} = 0. \tag{3}$$

One can approximate solution of Equation (3) with the third-degree piece-wise interpolation polynomial at time $k+1$ at every computational cell (i,j) as $\phi_{i,j}^{k+1} = P$ (see Figure 3 for positive u and v). Here,

$$P(\alpha,\beta) = \sum_{m=0}^{3}\sum_{n=0}^{3} \alpha^m \beta^n f_{m,n}, \tag{4}$$

$\alpha = u\Delta t/\Delta x = |x - x_i|/\Delta x$ and $\beta = v\Delta t/\Delta y = |y - y_j|/\Delta y$ are the Courant numbers in x and y directions; Δx, Δy are the respective cell dimensions; upper indexes m and n indicate power function; unknown components of vector $\mathbf{f} = \{f_{m,n}\}_{m,n=0,\ldots,3}$ have to be identified using some auxiliary conditions.

At this juncture one can choose the type of the polynomial approximation (4). As it was explored by Tkalich & Chan (2003), for maximum accuracy within the class of third-degree Lagrange polynomials one has to retain all 16 terms, and respectively, to have stencil consisting of the same number of nodes (components). Ten is the minimum number of terms (nodes or components) required to construct a 2-D third-order scheme having similar accuracy in x, y and xy (cross) directions; and twelve terms (nodes or components) were considered as optimal for the scheme efficiency. Using these findings, several 2-D extensions of QUICKEST algorithm have been derived and

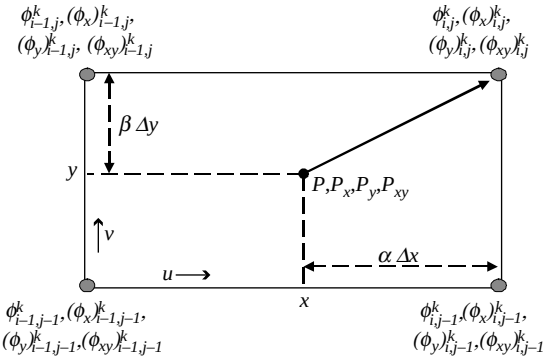

Figure 3 | Computational stencil.

written in a conservative form (Tkalich & Chan 2003)

$$\phi_{i,j}^{k+1} = \phi_{i,j}^{k} - \alpha((\phi_E)_{i,j} - (\phi_W)_{i,j}) - \beta((\phi_N)_{i,j} - (\phi_S)_{i,j}). \tag{5}$$

Here $(\phi_W)_i$, $(\phi_E)_i$, $(\phi_S)_i$, and $(\phi_N)_i$ are the west-, east-, south-, and north-face values of the transported scalar for the i-th cell. In order to construct Hermite polynomial approximation following Holly & Preissmann (1977) ideas, values of ϕ as well as its derivatives ϕ_x, ϕ_y and ϕ_{xy} have to be prescribed at the corners of i,j-th cell as shown in Figure 3. Newly introduced state variables ϕ_x, ϕ_y and ϕ_{xy} are governed by equation (3) differentiated with respect to x, y, and xy as

$$\frac{\partial \phi_x}{\partial t} + u\frac{\partial \phi_x}{\partial x} + v\frac{\partial \phi_x}{\partial y} = 0, \tag{6a}$$

$$\frac{\partial \phi_y}{\partial t} + u\frac{\partial \phi_y}{\partial x} + v\frac{\partial \phi_y}{\partial y} = 0, \tag{6b}$$

$$\frac{\partial \phi_{xy}}{\partial t} + u\frac{\partial \phi_{xy}}{\partial x} + v\frac{\partial \phi_{xy}}{\partial y} = 0. \tag{6c}$$

Expression (4) suggests solution of equations (6) as second-degree polynomials

$$P_x(\alpha,\beta) = \alpha_x \sum_{m=1}^{3}\sum_{n=0}^{3} m\alpha^{m-1}\beta^n f_{m,n}, \tag{7a}$$

$$P_y(\alpha,\beta) = \beta_y \sum_{m=0}^{3}\sum_{n=1}^{3} n\alpha^{m}\beta^{n-1} f_{m,n}, \tag{7b}$$

$$P_{xy}(\alpha,\beta) = \alpha_x\beta_y \sum_{m=1}^{3}\sum_{n=1}^{3} mn\alpha^{m-1}\beta^{n-1} f_{m,n}. \tag{7c}$$

Dougherty *et al.* (1989) iterated that the cubic Hermite interpolant is fourth-order accurate if the derivatives (P_x, P_y, and P_{xy}) are third-order, third-order if the derivatives are second order, etc. Hence, an algorithm of numerical treatment of derivatives (7) might improve or reduce the overall accuracy of the Holly-Preissmann method within the specified range.

To identify 16 components of vector $\mathbf{f}$ one has to assume that the polynomial P and its derivatives P_x , P_y, and P_{xy} satisfy transportivity properties (equations 3,6) at the computational stencil shown in Figure 3, leading to a

system of 16 linear equations

$$\begin{aligned}
&\phi^k_{i,j} = P(0,0), \phi^k_{i-1,j} = P(1,0), \phi^k_{i,j-1} \\
&\quad = P(0,1), \phi^k_{i-1,j-1} = P(1,1) \\
&(\phi_x)^k_{i,j} = P_x(0,0), (\phi_x)^k_{i-1,j} = P_x(1,0), (\phi_x)^k_{i,j-1} \\
&\quad = P_x(0,1), (\phi_x)^k_{i-1,j-1} = P_x(1,1) \\
&(\phi_y)^k_{i,j} = P_y(0,0), (\phi_y)^k_{i-1,j} = P_y(1,0), (\phi_y)^k_{i,j-1} \\
&\quad = P_y(0,1), (\phi_y)^k_{i-1,j-1} = P_y(1,1) \\
&(\phi_{xy})^k_{i,j} = P_{xy}(0,0), (\phi_{xy})^k_{i-1,j} = P_{xy}(1,0), (\phi_{xy})^k_{i,j-1} \\
&\quad = P_{xy}(0,1), (\phi_{xy})^k_{i-1,j-1} = P_{xy}(1,1)
\end{aligned} \tag{8}$$

System (8) can be solved with respect to vector components **f** which consequently need to be substituted into equations (4) and (7) to define single-step solutions of equations (3) and (6).

Due to a necessity to carry not only the transported scalar values, but also its spatial derivatives as depended variables in the Holly-Preissmann method, Komatsu *et al.* (1985) quoted it as "complicated and expensive" for 2-D applications. Indeed, utilizing ideas of Holly & Preissmann (1977) the 2-D algorithm has been obtained, where instead of solving single equation (3) one has to solve four equations (3), (6). To make it even more difficult, some environmental processes, such as eutrophication (Di Toro *et al.* 1983; Tkalich & Sundarambal 2003), might require 10 to 20 state variables with complex nonlinear right-hand-side functions describing mass exchange kinetics. The luxury of solving 40–80 equations for such environmental problems is seldom affordable. The Author still considers the Holly-Preissmann method to be very promising and important, but it needs to be reformulated in modern terms to be even more useful in many practical applications.

ACKNOWLEDGEMENTS

The Author wish to express sincere gratitude to the Discusser for raising fundamental comments which led to interesting and fruitful discussions.

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