Method of Characteristics for Pure Advection

By Gilberto E. Urroz, September 2004

Note: The following notes are based on class notes for the class COMPUTATIONAL HYDRAULICS, as taught by Dr. Forrest Holly in the Spring Semester 1985 at the University of Iowa.

Pure advection

The partial differential equation of pure-advection is

$$\frac{\partial c}{\partial t} + u\frac{\partial c}{\partial t} = 0,$$

where *u(x,t)* is the advection velocity, and *c(x,t)* represents the quantity being advected, e.g., a concentration of contaminant in a one-dimensional flow. This partial differential equation can be written also as an ordinary differential equation, namely,

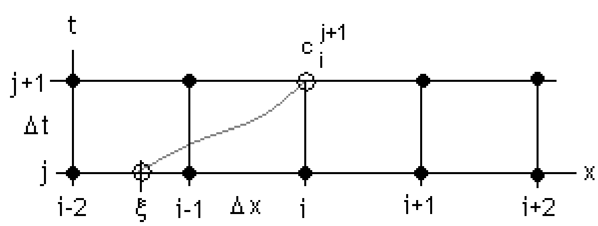
$$\frac{dc}{dt} = 0$$

along the characteristic curve $\frac{dx}{dt} = u(x,t)$.

Method of characteristics

The following computational grid illustrates the solution of the ODE *dc/dt = 0* along the characteristic curve *dx/dt = u*. We are interested in finding the value of $c_i^{j+1} = c(x_i, t_{j+1})$ along the characteristic curve that starts at position $x = \xi$ at time level *j*. Integrating *dc/dt = 0* along the trajectory illustrated in the figure produces simply:

$$\boxed{c_i^{j+1} = c_\xi}. \tag{C1}$$



To determine the value of ξ (i.e., the value of *x* at the foot of the trajectory) we can integrate the equation *dx/dt = u(x,t)* from point (ξ, t_j) to point (x_i, t_{j+1}), i.e.

$$\int_\xi^{x_i} dx = \int_{t_j}^{t_{j+1}} u(x,t)\,dt .$$

Integration along the characteristic curve produces the following result:

$$\xi = x_i - \int_{t_j}^{t_{j+1}} u(x,t)\,dt . \tag{T1}$$

For non-constant velocity *u(x,t)*, the integral in the previous equation can be approximated by

$$\int_{t_j}^{t_{j+1}} u(x,t)dt \approx \frac{1}{2}(u_i^{j+1} + u_\xi)\Delta t \, .$$

The expression for u_ξ, using a linear interpolation along x is:

$$u_\xi = u_{i-1}^j + \frac{\xi - x_{i-1}}{\Delta x_i}(u_i^j - u_{i-1}^j).$$

Replacing the last result into the previous equation, and that result, in turn, into equation (T1), produces

$$\boxed{\xi = \frac{x_i + \frac{\Delta t}{2\Delta x_i}(u_i^j - u_{i-1}^j)x_{i-1} - \frac{\Delta t}{2}(u_i^{j+1} + u_{i-1}^j)}{1 + \frac{\Delta t}{2\Delta x_i}(u_i^j - u_{i-1}^j)}}. \qquad \text{(T2)}$$

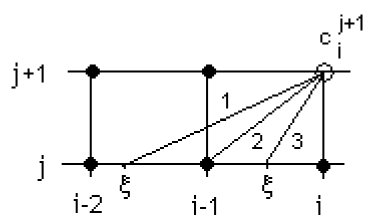
For the simple case in which *u(x,t) = constant*, the trajectory is a straight line:

$$\xi = x_i - u \cdot \int_{t_j}^{t_{j+1}} dt = x_i - u \cdot \Delta t = x_i - r \cdot \Delta x \, ,$$

where

$$\boxed{r = \frac{u \cdot \Delta t}{\Delta x}} \qquad \text{(R1)}$$

is the Courant number for the computational grid. The following figure illustrates three possible straight lines representing the characteristic curve for u = *constant*. For line 1, $r > 1$, and the foot of the line falls outside of the (i-1,i) cell. For line 2, r = 1, and the characteristic line is the cell's diagonal. Finally, for r<1 the foot of the characteristic line falls within the (i-1,i) cell.



Linear interpolation for concentration
Earlier on we found that the solution to the governing equation, namely, $dc/dt = 0$, along the characteristic curve is simply $c_i^{j+1} = c_\xi$. To determine the concentration at the foot of the trajectory, c_ξ, we can use a linear interpolation of the concentrations at points $i-1$ and i, at time level j, namely:

$$c_\xi = c_{i-1}^j + (1-r)(c_i^j - c_{i-1}^j) \, .$$

This simple linear interpolation approach works fine for $r = 1$ since no interpolation error is involved. In such case, $c_\xi = c_{i-1}^j$. However, the time step size Δt is constrained by u and Δx. If we adjust Δt so that $r>1$, c_ξ is calculated by extrapolating outside of the (i-1,i) cell which typically produces an unstable solution. On the other hand, if we adjust Δt so that $r<1$, linear interpolation will damp non-linear components of the solution.

In general, linear interpolation is not the best approach to estimate the concentration at the foot of the characteristic curve. Higher-order interpolation polynomials can improve the performance of the solution scheme. This approach is applied next in the *Holly-Preissmann scheme*.

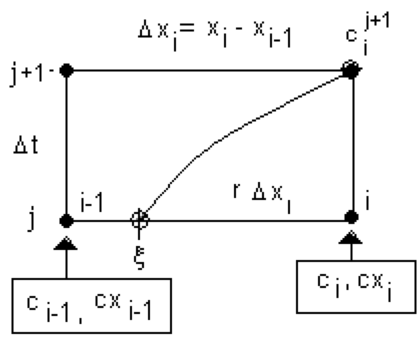
The Holly-Preissmann scheme
This method is based on constructing a third-order interpolating polynomial to calculate c_ξ based on the information from two points ($i-1,j$) and (i,j). The polynomial is written as

$$c(r) = A_1 + A_2\, r + A_3\, r^2 + A_4\, r^3, \tag{HP1}$$

where

$$\boxed{r = \frac{x_i - \xi}{\Delta x_i}}, \tag{R2}$$

and the A's are constant values. The meaning of the parameter r is illustrated in the figure below showing the characteristic line in a typical cell of the computational grid. (Note: for a constant value of u, the characteristic curve is a straight line and the parameter r is also the Courant number of the computational grid: $r = u{\cdot}\Delta t/\Delta x$).



In order to evaluate the constants of the cubic polynomial in equation (HP1), we would have to provide four values of *(r,c)*. However, since we have only two reference points where c is known, namely ($i-1,j$) and (i,j), we need to include also the derivative values cx = ∂c/∂x at those reference points. Notice that *cx* can be written in terms of r as follows:

$$cx = \partial c/\partial x = (dc/dr)(dr/dx) = c'(r)\ (-1/\Delta x_i).$$

Since, in the context of the calculation cell, $x = \xi$, the result $dr/dx = dr/d\xi = -1/\Delta x_i$ follows from equation (R2).

The equation to use for derivatives *cx* is, therefore,

$$cx(r) = -c'(r)/\Delta x_i = -(A_2 + 2A_3\, r + 3A_4\, r^2)/\Delta x_i. \tag{HP2}$$

The figure above illustrates the fact that the values c_{i-1}, cx_{i-1}, c_i, cx_i are known. These values correspond to $r = 1$ for $x = x_{i-1}$ and $r = 0$ for $x = x_i$. Thus, replacing the values of *c*, *cx*, and *r*, for points x_{i-1} and x_i, into equations (HP1) and (HP2), produce a system of linear equations whose solution is given by

$A_1 = c_i,$
$A_2 = -\Delta x_i\, cx_i,$
$A_3 = (2cx_i + cx_{i-1})\Delta x_i + 3(c_{i-1}-c_i),$
$A_4 = -(cx_i + cx_{i-1})\Delta x_i + 2(c_i-c_{i-1}).$

Replacing these constants into equation (HP1) and collecting terms allows us to re-write equation (HP1) as

$$c(r) = a_1\, c_{i-1} + a_2\, c_i + a_3\, cx_{i-1} + a_4\, cx_i, \qquad \text{(HP3)}$$

where

$a_1 = r^2(3-2r)$
$a_2 = 1- \ r^2(3-2r) = 1 - a_1,$
$a_3 = r^2(1-r)\Delta x_i,$
$a_4 = - r(1-r)^2.$

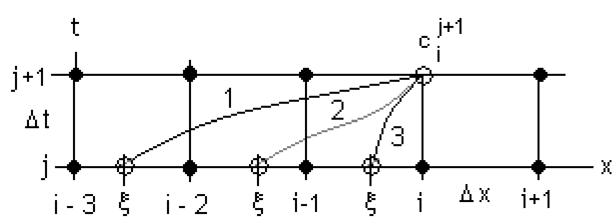
Also, equation (HP2) now becomes

$$cx(r) = b_1\, c_{i-1} + b_2\, c_i + b_3\, cx_{i-1} + b_4\, cx_i, \qquad \text{(HP4)}$$

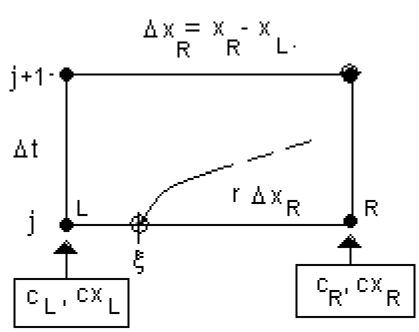
where

$b_1 = 6r(1-r)/\Delta x_i$
$b_2 = 6r(r-1)/\Delta x_i = - b_1,$
$b_3 = r(3r-2)\Delta x_i,$
$b_4 = (r-1)(3r-1).$

Notice that this solution assumes that $x=\xi$ is such that $x_{i-1} < \xi < x_i$, as in line 3 in the figure below. It may happen, however, that the foot of the trajectory to point (x_i,t_j) falls in a cell to the left of $[x_{i-1},x_i]$ as illustrated by lines 1 and 2 in the figure below.



The solutions for *c(r)* and *cx(r)* provided by equations (HP3) and (HP4), respectively, can be applied to any cell regardless of whether ξ is within the range $[x_{i-1},x_i]$ or in a cell to the left of this range. The figure below illustrates the situation for any interval $[x_L,x_R]$. (NOTE: for line 1 in the figure above, $R = i-2$, $L = i-3$, etc.)



Thus, regardless of which cell the value of *x* falls into, the interpolating polynomials can be written as:

$$\boxed{c(r) = a_1 c_L + a_2 c_R + a_3 cx_L + a_4 c_R}, \qquad \text{(HP5)}$$

where

$a_1 = r^2(3-2r)$
$a_2 = 1- \ r^2(3-2r) = 1 - a_1,$
$a_3 = r^2(1-r)\Delta x_R,$
$a_4 = - r(1-r)^2.$

Also, equation (HP2) now becomes

$$\boxed{cx(r) = b_1 c_L + b_2 c_R + b_3 cx_L + b_4 cx_R}, \qquad \text{(HP6)}$$

where

$b_1 = 6r(1-r)/\Delta x_R$
$b_2 = 6r(r-1)/\Delta x_R = - b_1,$
$b_3 = r(3r-2)\Delta x_R,$
$b_4 = (r-1)(3r-1).$

In these expressions, $\boxed{\Delta x_R = x_R-x_L}$.

Advecting cx = ∂c/∂x

While the Holly-Preissmann scheme provides a more stable approach to the problem of pure advection of the concentration *c(x,t)*, it also requires the advection of the derivatives cx = ∂c/∂x. An advection equation for *cx* can be obtained by taking the derivative of the advection equation with respect to x so that we can write

$$\frac{\partial}{\partial t}cx + u\frac{\partial}{\partial t}cx = -cx \cdot \frac{\partial u}{\partial x}.$$

This result is equivalent to solving

$$\frac{dc}{dt} = -cx \cdot \frac{\partial u}{\partial x},$$

along the trajectory $\frac{dx}{dt} = u(x,t)$.

Integration of the ordinary differential equation for cx, along the trajectory, results in

$$cx_i^{j+1} = cx_\xi - \int_{t_j}^{t_{j+1}} cx \cdot \frac{\partial u}{\partial x} \cdot dt .$$

The value of $cx_\xi = cx(r)$ is calculated with equation (HP4), while the integral in the right-hand side is approximated by the trapezoidal rule:

$$-\int_{t_j}^{t_{j+1}} cx \cdot \frac{\partial u}{\partial x} \cdot dt = -\frac{t_{j+1}-t_j}{2} \cdot \left(cx_\xi \cdot \frac{\partial u}{\partial x}\Big|_{\xi,j} + cx^{j+1}_i \cdot \frac{\partial u}{\partial x}\Big|_{i,j+1} \right).$$

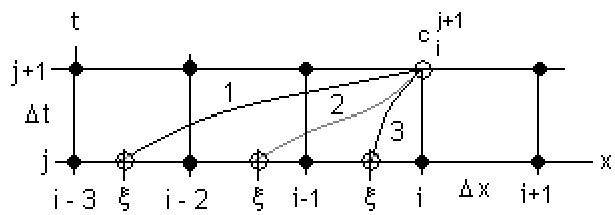
Replacing this result in the previous equation and solving for cx_i^{j+1} results in:

$$cx_i^{j+1} = cx_\xi \cdot \left(\frac{1 - \frac{\Delta t}{2} \frac{\partial u}{\partial x} |_{\xi,j}}{1 + \frac{\Delta t}{2} \frac{\partial u}{\partial x} |_{i,j+1}} \right). \quad \text{(C2)}$$

Notice that, if $u = constant$, $\partial u/\partial x = 0$, and $cx_i^{j+1} = cx_\xi$. For non-constant $u(x,t)$, the values of $\partial u/\partial x$ at points (ξ,j) and $(i,j+1)$ can be estimated with finite differences and interpolation since the velocity field $u(x,t)$ is supposed to be known. The following formulations can be used to calculate the derivatives $\partial u/\partial x$ shown in equation (C2). The derivative at point $(i,j+1)$ can be determined as

$$\left.\frac{\partial u}{\partial x}\right|_{i,j+1} \approx \frac{u_i^{j+1} - u_{i-1}^{j+1}}{\Delta x_i}. \quad \text{(DU1)}$$

To estimate the derivative $\partial u/\partial x$ at point (ξ,j), we need to take into consideration the fact that the foot of the trajectory, ξ, may fall in the interval $[x_{i-1},x_i]$ or in any of the intervals to the left, as illustrated in the following figure.



Thus, once the interval where ξ is located has been identified, we can estimate the derivative at that point as

$$\left.\frac{\partial u}{\partial x}\right|_{\xi,j} \approx \frac{u_R^j - u_\xi^j}{x_R - \xi}. \quad \text{(DU2)}$$

In this formulation, R stands for the index of the right-side limit of the interval where ξ is located. For example, referring to the figure immediately above, for characteristic line 1, $R = i-2$. Similarly, for line 2, $R = i-1$, and for line 3, $R = i$.

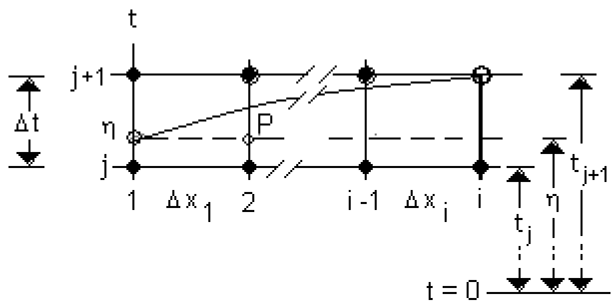
If the values of the velocity $u(x,t)$ are only known at the nodes of the calculation grid, it will be necessary to interpolate u_ξ^j from the known node values, say, u_R^j and u_L^j. (Here, R and L stand for the indices of the right-side and left-side limits, respectively, of the interval where ξ is located. Thus, in the figure immediately above, for lines 1, 2, and 3, $L = i-3$, $i-2$, and $i-1$, respectively.) Simple linear interpolation of u along x reveals that

$$\frac{u_R^j - u_\xi^j}{x_R - \xi} = \frac{u_R^j - u_L^j}{x_R - x_L},$$

therefore, the derivative $\partial u/\partial x$ at point (ξ,j), can be calculated as:

$$\boxed{\left.\frac{\partial u}{\partial x}\right|_{\xi,j} \approx \frac{u_R^j - u_L^j}{x_R - x_L} = \frac{u_R^j - u_L^j}{\Delta x_R}}. \qquad \text{(DU3)}$$

Consider the case in which the characteristic curve starts at point x_3 or larger, but it hits the first cell along the *t* axis at a point η such that $t_j < \eta < t_{j+1}$. This case is illustrated in the figure below.



To determine the value $t = \eta$, where the characteristic curve hits the line $x = x_1$, we integrate the characteristic curve, $dx/dt = u$, between points η and *(i,j+1)*. The result is:

$$x_i - x_1 = \int_{\eta}^{t_{j+1}} u dt \approx \frac{1}{2}(u_i^{j+1} + u_\eta)(t_{j+1} - \eta).$$

Linear interpolation of the velocity with time at location $x=x_1$ indicates that

$$u_\eta = u_1^j + \frac{\eta - t_j}{t_{j+1} - t_j}(u_1^{j+1} - u_1^j) = u_1^j + \frac{\eta - t_j}{\Delta t_j}(u_1^{j+1} - u_1^j).$$

Replacing this expression for u_η in the equation for $x_i - x_1$, and performing some algebraic manipulation, produces a quadratic equation in η:

$$\boxed{M_1\eta^2 - M_2\eta + M_3 = 0}, \qquad \text{(ETA1)}$$

where

$$M_1 = \frac{u_1^{j+1} - u_1^j}{2\Delta t},$$

$$M_2 = \frac{u_1^{j+1} - u_1^j}{2\Delta t}(t_j + t_{j+1}) - \frac{u_2^{j+1} + u_1^j}{2},$$

and

$$M_3 = x_i - x_1 + \frac{u_{i-1}^{j+1} - u_{i-1}^j}{2\Delta t} \cdot t_j \cdot t_{j+1} - \frac{u_i^{j+1} + u_{i-1}^j}{2} \cdot t_{j+1}.$$

There are two possible solutions for η from the quadratic equation shown above. The solution of interest is the value of η for which $t_j < \eta < t_{j+1}$.

If the case described above arises in a solution, it will be necessary to calculate the following derivative to perform the advection of $cx = \partial c/\partial x$:

$$\left.\frac{\partial u}{\partial x}\right|_{\eta,j} \approx \frac{u_P - u_\eta}{x_2 - x_1} = \frac{u_P - u_\eta}{\Delta x_2},$$

where point P corresponds to $t = \eta$ and $x = x_2$. In the figure above, η is the foot of the characteristic trajectory leading to point (x_i, t_{j+1}). The value u_P can be obtained by linear interpolation with respect to t, namely,

$$u_P = u_2^j + \frac{\eta - t_j}{t_{j+1} - t_j}(u_2^{j+1} - u_2^j) = u_2^j + \frac{\eta - t_j}{\Delta t_j}(u_2^{j+1} - u_2^j).$$

With the expressions for u_P and u_η found above, the derivative $\partial u/\partial x$ at point (η, j), is now written as

$$\boxed{\left.\frac{\partial u}{\partial x}\right|_{\eta,j} \approx \alpha_t\left(\frac{u_2^{j+1} - u_1^{j+1}}{\Delta x_2}\right) + (1-\alpha_t)\left(\frac{u_2^j - u_1^j}{\Delta x_2}\right)}, \tag{DU4}$$

where

$$\boxed{\alpha_t = \frac{\eta - t_j}{\Delta t_j}}.$$

The equation for calculating cx_i^{j+1} for this particular situation is:

$$\boxed{cx_i^{j+1} = cx_\eta \cdot \left(\frac{1 - \frac{\Delta t}{2}\frac{\partial u}{\partial x}|_{\eta,j}}{1 + \frac{\Delta t}{2}\frac{\partial u}{\partial x}|_{i,j+1}}\right)}. \tag{C3}$$

Note: the derivative $\partial u/\partial x$ at point $(i, j+1)$ can be determined as in equation (DU1).

Initial conditions

The initial conditions for the concentration and its derivative in x are simply values of $c_i^{j=1} = c(x_i, t_1)$ and $cx_i^{j=1} = cx(x_i, t_1)$. These values should be known. If only the values of c_i^1 are given, the values of $cx_i^1 = \partial c/\partial x|_{t1}$ can be obtained using finite-differences, e.g.,

$$\boxed{cx_i^1 = \frac{c_{i-1}^1 - c_{i+1}^1}{2\Delta x}},$$

for $i = 2, 3, \ldots, n$, and

$$\boxed{cx_i^1 = \frac{c_2^1 - c_i^1}{\Delta x},\ cx_{n+1}^1 = \frac{c_{n+1}^1 - c_n^1}{\Delta x}}.$$

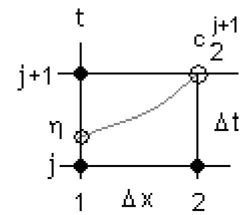
These results apply to a solution domain with n sub-intervals of length $\boxed{\Delta x = L/n}$, where L is the length of the reach of interest along the x direction. The grid points in x are calculated with

$$\boxed{x_i = (i-1)\Delta x},$$

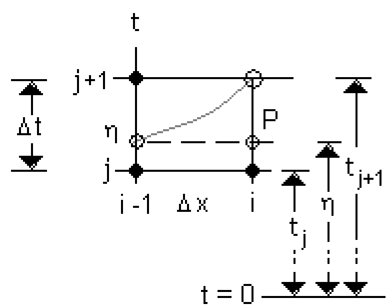
for $i = 1, 2, \ldots, n+1$.

Boundary conditions
Only the upstream boundary condition is needed. The simplest case is when values of both $c_1(t) = c_1^j = c(x_1,t)$ and $cx_1(t) = cx_1^j = \partial c/\partial x|_{1,t}$ are provided. Alternatively, only the values of $c_1(t)$ are provided. This last case is discussed later in this section. Next, we analyze a possible situation assuming that both $c_1(t)$ and $cx_1(t)$ are given.

The possibility exists that at the upstream boundary the parameter r is larger than 1. This situation is illustrated by the figure below. The issue in this case is to be able to determine the value $t = \eta$ where the characteristic curve hits the line $x = x_1$, and then find the values $c_\eta = c(x_1,\eta)$, and $cx_\eta = cx(x_1,\eta)$.



The following figure is used to develop an algorithm for determining the value of $t = \eta$. Although the grid shown applies to any value of i, the approach is to be used exclusively in the upstream boundary, i.e., for $i = 2$.



To determine the value $t = \eta$, where the characteristic curve hits the line $x = x_{i-1}$, we can integrate the characteristic curve, $dx/dt = u$, between points η and $(i,j+1)$. The result is:

$$\Delta x_i = x_i - x_{i-1} = \int_{t_\eta}^{t_{j+1}} u dt \approx \frac{1}{2}(u_i^{j+1} + u_\eta)(t_{j+1} - \eta)\,.$$

Linear interpolation of the velocity with time at location $x=x_{i-1}$ indicates that

$$u_\eta = u_{i-1}^j + \frac{\eta - t_j}{t_{j+1} - t_j}(u_{i-1}^{j+1} - u_{i-1}^j) = u_{i-1}^j + \frac{\eta - t_j}{\Delta t_j}(u_{i-1}^{j+1} - u_{i-1}^j)\,.$$

Replacing this expression for u_η in the equation for Δx_i, and performing some algebraic manipulation, produces a quadratic equation in η, namely:

$$\boxed{K_1\eta^2 - K_2\eta + K_3 = 0}, \qquad \text{(ETA1)}$$

where

$$K_1 = \frac{u_{i-1}^{j+1} - u_{i-1}^j}{2\Delta t}\,,$$

$$K_2 = \frac{u_{i-1}^{j+1} - u_{i-1}^{j}}{2\Delta t}(t_j + t_{j+1}) - \frac{u_i^{j+1} + u_{i-1}^{j}}{2},$$

and

$$K_3 = \Delta x_i + \frac{u_{i-1}^{j+1} - u_{i-1}^{j}}{2\Delta t} \cdot t_j \cdot t_{j+1} - \frac{u_i^{j+1} + u_{i-1}^{j}}{2} \cdot t_{j+1}.$$

There are two possible solutions for η from the quadratic equation shown above. The solution of interest is the value of η for which $t_j < \eta < t_{j+1}$.

If the case $r>1$ arises in the upstream boundary, it will be necessary to calculate the following derivative to perform the advection of $cx = \partial c/\partial x$:

$$\left.\frac{\partial u}{\partial x}\right|_{\eta,j} \approx \frac{u_P - u_\eta}{x_i - x_{i-1}} = \frac{u_P - u_\eta}{\Delta x_i},$$

where point P corresponds to $t = \eta$ and $x = x_i$. In the figure above, η is the foot of the characteristic trajectory leading to point (x_i, t_{j+1}). The value u_P can be obtained by linear interpolation with respect to t, namely,

$$u_P = u_i^j + \frac{\eta - t_j}{t_{j+1} - t_j}(u_i^{j+1} - u_i^j) = u_i^j + \frac{\eta - t_j}{\Delta t_j}(u_i^{j+1} - u_i^j).$$

With the expressions for u_P and u_η found above, the derivative $\partial u/\partial x$ at point (η, j), is now written as

$$\boxed{\left.\frac{\partial u}{\partial x}\right|_{\eta,j} \approx \alpha_t\left(\frac{u_i^{j+1} - u_{i-1}^{j+1}}{\Delta x_i}\right) + (1-\alpha_t)\left(\frac{u_i^j - u_{i-1}^j}{\Delta x_i}\right)}, \quad \text{(DU4)}$$

where α_t was defined earlier.

The equation for calculating cx_i^{j+1} for this particular situation is equation (C3) with $i = 2$. The derivative $\partial u/\partial x$ at point $(i, j+1)$, needed in (C3), is determined as in equation (DU1) with $i = 2$. Recall that this approach is only needed if $\xi < x_1$ (i.e., if ξ falls to the left of the upper-boundary cell), therefore, it is only used with $i = 2$.

If only the values of $c_1(t)$ are provided, it is possible to calculate the values of cx_i^1 as follows:

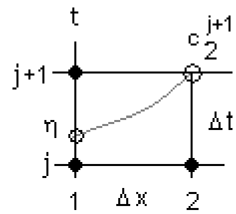
$$\boxed{cx_i^1 = \frac{c_{i-1}^1 - c_{i+1}^1}{2\Delta x}},$$

for $i = 2, 3, \ldots, n$, and

$$\boxed{cx_1^1 = \frac{c_2^1 - c_1^1}{\Delta x},\ cx_{n+1}^1 = \frac{c_{n+1}^1 - c_n^1}{\Delta x}}.$$

Assuming that none of the characteristic lines ever hit the t axis (i.e., there is no need to determine point (x_1, η) as the foot of one or more characteristic lines), then, the procedure is straightforward, with the numerical solution advecting the values of c_i^1 and cx_i^1 in time.

If the case occurs that a characteristic hits the t axis, as illustrated in the figure below, it will be necessary to determine the value of cx_1^2 numerically. We only need to do this with the first characteristic that hits the t axis, since we will be using a third order polynomial in t to interpolate values of c and of cx for $x=x_1$ and $t_j < \eta < t_{j+1}$. Any other characteristic that starts at the t axis will have values of c_η and cx_η interpolated from the known cubic polynomial.



Let the curve starting at (x_1,η) and ending at point (x_2,t_{j+1}), as shown above, be the first characteristic curve that hits the t axis for the period $t_j < t < t_{j+1}$. The values of c_1^j and c_1^{j+1} are known, and the value of cx_1^j has been calculated with

$$cx_1^j = \frac{c_2^j - c_1^j}{\Delta x}.$$

As a first approximation to c_η we use a linear interpolation on t, namely,

$$c_2^{j+1} = c_\eta = c_1^j + \frac{\eta - t_j}{t_{j+1} - t_j}(c_1^{j+1} - c_1^j) = c_1^j + \frac{\eta - t_j}{\Delta t_j}(c_1^{j+1} - c_1^j).$$

Then, we can estimate cx_1^{j+1} as

$$cx_1^{j+1} = \frac{c_2^{j+1} - c_1^{j+1}}{\Delta x}. \qquad \text{(C3)}$$

The interpolating polynomials for $c(t)$ at $x=x_1$ are given by

$$c(r) = \alpha_1 c^{j-1} + \alpha_2 c^j + \alpha_3 cx^{j-1} + \alpha_4 cx^j, \qquad \text{(HP7)}$$

$\alpha_1 = s^2(3-2s)$
$\alpha_2 = 1- s^2(3-2s) = 1 - \alpha_1,$
$\alpha_3 = s^2(1-s)\Delta x_i,$
$\alpha_4 = - s(1-r)^2.$

and,

$$cx(r) = \beta_1 c^{j-1} + b_2 c^j + b_3 cx^{j-1} + b_4 cx^j, \qquad \text{(HP8)}$$

$\beta_1 = 6s(1-s)/\Delta x_i$
$\beta_2 = 6s(s-1)/\Delta x_i = - b_1,$
$\beta_3 = s(3s-2)\Delta x_i,$
$\beta_4 = (s-1)(3s-1).$

In both equations (HP7) and (HP8), the value of s represents

$$\boxed{s = \frac{t_{j+1} - \eta}{\Delta t_i} = \alpha_t}. \quad \text{(S1)}$$

To improve the calculation of cx_1^{j+1} an iterative process can be implemented by which a new estimate of $c_h = c_2^{j+1}$ is calculated with equation (HP7), then a new estimate of cx_1^{j+1} is calculated with equation (C3). The iteration continues until two consecutive values of cx_1^{j+1} are within a margin of error ε, i.e., until

$$|(cx_1^{j+1})_{k+1} - (cx_1^{j+1})_k| < \varepsilon .$$

Implementation of numerical solution

The following is an outline of the algorithm for the numerical solution of the pure-advection equation utilizing the Holly-Preissmann scheme:

1. Apply initial conditions to load values of $c_i^{j=1}$ and $cx_i^{j=1}$ for all values of i.

For every time step (say, $j = 2, 3, \ldots, m$) and for every inner x point (say, $i = 2, 3, \ldots, n$):

2. Compute trajectory from x_i at time level $j+1$ back to ξ at time level j by using equation (T2).
3. Construct the interpolating polynomials for $c(r)$ and $cx(r)$ as defined by equations (HP5) and (HP6). Basically, you need to calculate the coefficients in the polynomials, namely, $a_1, a_2, \ldots, b_1, b_2, \ldots$.

4. Calculate r with equation (R2), determine the values of the index R and L (by determining the interval $[x_{i-1},x_i]$, where ξ is located, i.e., $R = i$ and $L = i-1$ if $x_{i-1} < \xi < x_i$), and evaluate $c(r)$ and $cx(r)$ with the coefficients calculated in step 3.

5. Compute $c_i^{j+1} = c_\xi$ and cx_i^{j+1} from equation (C2). The derivatives $\partial u/\partial x$ required in equation (C2) can be calculated using equations (DU1), and one of equations (DU2), (DU3), or (DU4). [NOTE: equation (DU4) is only needed in the upstream boundary cell if $r>1$, and the determination of $t = \eta$ at $x=x_1$, from equation (ETA1), is required – see step 6, below].

6. Apply upstream boundary condition to load c_1^{j+1} and cx_1^{j+1}. Write the code to account for all possible cases as outlined in the section on the boundary conditions.

Exercise – Modeling the pure advection of a Gaussian contaminant distribution

Consider a Gaussian distribution of contaminant given by the equation

$$c_0(x) = 10 \cdot \exp\left(-\frac{(x - x_o)^2}{2\sigma_x^2} \right),$$

with $\sigma_x = 264\ m$. Use this equation to provide the initial and boundary conditions for a pure-advection simulation in a channel that is *10-km* long (L = 10 km) if the simulation lasts for $t_{max} = 160$ *minutes*. The water in the channel is moving with a constant velocity $u = 0.5\ m/\text{s}$. At time $t = 0$, the curve is centered at $x_0 = 0$ (initial conditions), and, for $t>0$, the lagging half of the distribution enters the model as the boundary condition $c_1(t)$. (a) Write a *Matlab* function to implement the numerical solution of pure advection using the Holly-Preissmann algorithm. (b) Use a script to perform to activate the function and perform the pure-advection simulation with Δx = *200 m*, and Δt = *100 s, 200 s, 300 s, 400 s,* and *800 s*. Let the script also plot solution curves *c* vs. *t* for the different values of Δt at *t = 800 s, 1600 s, 2400 s*, and so on, until reaching t_{max}. Also, plot the exact solution (i.e., the advection of the Gaussian curve at a constant speed *u*) for the times indicated above in the same graphs. (c) Repeat one of the calculations in (b), but this time set *c = 0* at time *t = 0* (i.e., $c_0(x) = 0$). Discuss the effect of this inconsistency in the results.