A

Solution of the Advection-Diffusion Transport Equation using the Total Derivative and Least Squares Collocation

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INTRODUCTION

The difficulties arising in the application of numerical approximations to advection-diffusion transport problems are well known. The difficulties arise because of the dual nature of the equation. When the transport is advection dominated, the equation behaves as a first order equation. When the transport is diffusion dominated, the equation behaves as a second order parabolic equation.

Recently many workers have turned to Eulerian-Lagrangian methods (ELM) in an attempt to satisfactorily capture both the second order parabolic and first order nature of the equation (Baptista (1987), Glass and Rodi (1982), Holly and Polatera (1984) and Neuman (1984)). The equation is solved in two steps. In the first step, past information is carried along characteristics, thereby decoupling the solution of the first order part of the equation from the second order parabolic part. In the second step, the second order parabolic problem is solved on a fixed grid.

The following method resembles an ELM in that information that is required in the difference equations will be brought from the last time step by tracking along characteristics. The advection-diffusion equation is written in Lagrangian coordinates. It is then approximated by a central difference in time and a least squares collocation (LESCO) (Joos, 1986) discretization in space. It is the collocation point locations which are backward projected along characteristics. A major difference between our approach and ELMs is that no intermediate solution is computed.

DEVELOPMENT

In a Lagrangian system, the one dimensional advection-diffusion tran sport equation is written:

$$\frac{DC(x,t)}{Dt} + LC(x,t) = 0 \tag{1}$$

$$+.5\mathrm{L}\left\{\sum_{i=1}^{nbas}\alpha_i(t_n)\Phi_i(x_k)\right\}+.5\mathrm{L}\left\{\sum_{i=1}^{nbas}\alpha_i(t_{n-1})\Phi_i(x_k^*)\right\} \tag{4}$$

R_k is the residual associated with the k^{th} collocation point. When the collocation point comes from a location within the domain of the last time step, the function and the operator of the last time step are simply evaluated from the cubic approximating function of the last time step at that location.

When the flow line intersects the domain boundary, the evaluation of the function and operator of the last time step is more complicated. If t_i is the time of intersection and x_B is the boundary coordinate, then Δt of Eq. (2) becomes $t_n - t_i$, x_k^* becomes x_B and $\dot{C}(x_k^*,t_{n-1})$ becomes $C(x_B,t_i)$. The values of $C(x_B,t_i)$ and $\mathrm{L}C(x_B,t_i)$ must be approximated. If the boundary condition is of the first type, then $C(x_B,t_i)$ is simply the boundary value at time t_i . The spatial operator is approximated by:

$$\mathrm{L}\hat{C}(x_B,t_i) = \beta\mathrm{L}\hat{C}(x_k,t_n)+(1-\beta)\mathrm{L}\hat{C}(x_B,t_{n-1}) \tag{5}$$

where:

$$\beta = \frac{t_i - t_{n-1}}{\Delta t}$$

Substitution of Eqs. (3) and (5) into Eq. (2) yields the error, R_k , associated with a collocation point that entered the domain during the last time step:

$$R_k = \frac{1}{t_n - t_i}\sum_{i=1}^{nbas}\alpha_i(t_n)\Phi_i(x_k) - \frac{\hat{C}(x_B,t_i)}{t_n - t_i} + .5(1+\beta)\mathrm{L}\left\{\sum_{i=1}^{nbas}\alpha_i(t_n)\Phi_i(x_k)\right\}$$

$$+.5(1-\beta)\mathrm{L}\left\{\sum_{i=1}^{nbas}\alpha_i(t_{n-1})\Phi_i(x_B)\right\} \tag{6}$$

t_i never equals t_n, but as it approaches t_n, the formulation approaches fully implicit. As t_i approaches t_{n-1} the formulation approaches Crank Nicolson.

The sum of the squares of all of the errors, ε , is:

$$\varepsilon = \sum_{k=1}^{ncol} R_k^2 \tag{7}$$

where *ncol* is the number of collocation points.

To minimize the sum of the squares of the errors, the derivatives with respect to the coefficients $\alpha_j(t)$ are set equal to zero:

$$\frac{\partial\varepsilon}{\partial\alpha_j(t_n)} = 2\sum_{k=1}^{ncol} R_k \frac{\partial R_k}{\partial\alpha_j(t_n)} = 0 \qquad j = 1,nbas \tag{8}$$

Combination of Eqs. (4), (6), and (8) yields the least squares collocation set of equations:

$$\left\{\sum_{k=1}^{ncol}\sum_{i=1}^{nbas}\mathrm{L}_1\Phi_i(x_k)\mathrm{L}_1\Phi_j(x_k)\right\}\alpha_i(t_n) = \sum_{k=1}^{ncol}\mathrm{L}_1\Phi_j(x_k)\sum_{i=1}^{nbas}\mathrm{L}_2\Phi_i(x_k^*)\,\alpha_i(t_{n-1}) \tag{9}$$

$$for \qquad j = 1,nbas$$

The form of the operators L_1 and L_2 varies depending on the location of the backward projected collocation point. When the collocation point comes from within the domain of the last time step, the use of Eq. (4) yields:

$$L_1 = \frac{1}{\Delta t} + .5L \tag{9a}$$

$$L_2 = \frac{1}{\Delta t} - .5L \tag{9b}$$

When the collocation point enters the domain from the first type boundary at x_B and at time t_i, then Eq. (6) yields:

$$L_1 = \frac{1}{t_n - t_i} + .5(1+\beta)L \tag{9c}$$

$$\sum_{i=1}^{nbas} L_2\Phi_i(x_k^*)\,\alpha(t_{n-1}) = \frac{C(x_B,t_i)}{t_n - t_i} - .5(1-\beta)\sum_{i=1}^{nbas} L\Phi_i(x_B)\alpha_i(t_{n-1}) \tag{9d}$$

Cubic Hermites allow the specification of both the function and the first derivative at each node. Consequently, boundary conditions of both the first and second type are directly enforced in the matrix equations. The initial conditions are imposed by least squares fitting the cubic hermites to the initial values of concentration at the collocation points.

In summary, the computations required for each time step are:

1. Choose the collocation point locations (x_k) of the time step to be computed.
2. Back project the collocation point locations to the last time step (i.e., compute x_k^*).
3. Compute the coefficient matrix and the right hand side vector using Eq. (9).
4. Solve the matrix equation for $\alpha_i(t_n)$.
5. Compute the new set of C^1 continuous cubic polynomials that approximate the solution at the present time step by summing over all of the base functions in each element.

RESULTS

The results of two simulations are presented in Figures 1 and 2. In both cases velocity = .5, time increments = 192, total time steps = 50, element lengths = 200 and there are 8 collocation points per element. The Courant number is 0.48. Analytic solutions are solid lines and LESCO computed solutions are dash-double dot lines. The oscillatory Galerkin finite element solutions are shown as dash-dot lines. The Galerkin solution used Lagrange quadratic basis functions with element lengths of 200 and node spacing of 100.

In Figure 1, the diffusion coefficient is zero (the pure advection case) and a gaussian plume of standard deviation 264 was used as the initial condition. The right boundary has a zero concentration, and the left boundary a zero derivative. The analytic and LESCO computed solutions are coincident.

. In Figure 2, a concentration front is propagated from the left boundary. The initial condition was zero concentration. The left boundary concentration is one, and the right boundary derivative is zero. The diffusion coefficient is one, and the grid Peclet number is 100. The analytic and LESCO computed solutions are essentially coincident.

CONCLUSION

Excellent results have been obtained using the total derivative and LESCO to solve the advection-diffusion transport equation. As can be seen from the two examples, the method works well in advection dominated transport. This is partially due to having eliminated the first order hyperbolic term that dominates when the Peclet number is large. In addition, numerical test results, not presented here, have demonstrated that the LESCO formulation reproduces the higher spatial frequencies in the concentration fronts in a superior way. As the velocity decreases, the equations reduce to the Eulerian equations for diffusion, so the procedure works well for diffusion dominated transport as well. Given the promising early results, the method deserves further investigation.

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