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One stabilization method for the 1-D steady solute transport equation

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Abstract

The aim of this paper is to obtain a stabilized solution of the solute transport equation, as described in references such as Oñate [1] among others. The solution obtained by means of either finite element or finite volume methods may have undesirable oscillations (this may happen if, for example, the Peclet number id high). Those oscillations may be avoided by implementing stabilization techniques, as the one described in this paper. It consists of modifying the original partial differential equation (PDE) by considering higher order terms in the Taylor expansions, which is equivalent to introduce a certain amount of *artificial diffusion* in de convective and diffusive terms. This problem is then solved by the application of finite volumes, in order to obtain an approached solution, which is then substituted in the original PDE to aobtain a residual, which must be minimized by means of an iterative method. This iterative method keeps on, until a suffiently stable solution is achieved. Results are shown when the method es applied to velocity fields and diffusive coefficients strongly depending on the spatial coordinate.

Key words: Solute transport equation, stabilization
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1 Boundary problem formulation

The 1-D solute transport boundary problem is formulated as:

$$\frac{\partial(a(x,t)\cdot U(x,t))}{\partial t} + \frac{\partial}{\partial x}\left(v(x,t)\cdot U(x,t) - K(x,t)\frac{\partial U(x,t)}{\partial x}\right) + q(x,t)\cdot U(x,t) = f(x,t)$$

(+ boundary conditions and initial conditions)

where x is the spatial coordinate, t is the time, $U(x,t)$ is the unknown (mass concentration), $a(x,t)$ is the retardation factor, $v(x,t)$ is the velocity field, $K(x,t)$ is the dispersion-diffusion coefficient, $q(x,t)$ is a reaction coefficient and $f(x,t)$ is the source term.

When referring to the steady-state, the previous equation takes the form:

$$\frac{d}{dx}\left(v(x)\cdot U(x) - K(x)\frac{dU(x)}{dx}\right) + q(x)\cdot U(x) = f(x) \tag{1}$$

with the addition of boundary conditions.

This boundary problem may be solved by means of several well-known techniques such as: finite difference, finite element or finite volume methods. Whichever technique be used, an approached solution is achieved.

In this work, a finite volume technique is used. This method requires the problem to be formulated as a conservation law,as it will be explained below.

2 Finite volume scheme

In order to apply a finite volume scheme to the 1-D boundary problem (1), let us consider an interior domain, $S = [S_i, S_d]$, within Ω. Integration of (1) over the domain S yields:

$$-\int_S \frac{d}{dx}\left(K(x)\frac{dU(x)}{dx}\right)dx + \int_S \frac{d}{dx}\left(v(x)\cdot U(x)\right)dx + \int_S q(x)\cdot U(x)\,dx = \int_S f(x)\,dx \tag{2}$$

By direct integration of the convective-diffusive term, expression (2) may be re-written as:

$$\left(-K(x)\frac{dU(x)}{dx} + v(x)\cdot U(x)\right)_{S_i} - \left(-K(x)\frac{dU(x)}{dx} + v(x)\cdot U(x)\right)_{S_d} + \int_S q(x)\cdot U(x)\,dx = \int_S f(x)\,dx \tag{3}$$

The leading idea of the finite volume methods consists of estimating the exact solution $U(x)$ by means of an approaching function $\varphi(x)$, whose restriction to the sub-domain S will be denoted as $\varphi_S(x)$. First of all, we oblige this function to satisfy the equation (3):

$$\left(-K(x)\frac{d\varphi_S(x)}{dx} + v(x)\cdot \varphi_S(x)\right)_{S_i} - \left(-K(x)\frac{d\varphi_S(x)}{dx} + v(x)\cdot \varphi_S(x)\right)_{S_d} + \int_S q(x)\cdot \varphi_S(x)\,dx = \int_S f(x)\,dx$$

The flux between two neighbour sub-domains must conserve, hence, if we consider two adjacent intervals: $S = [S_i, S_d]$ and $S' = [S'_i, s?_d]$, where $S_d \equiv S'_i$, the fluxes must verify:

$$\left(-K(x)\frac{d\varphi_S(x)}{dx} + v(x)\cdot \varphi_S(x)\right)_{S_d} \equiv \left(-K(x)\frac{d\varphi_S(x)}{dx} + v(x)\cdot \varphi_S(x)\right)_{S'_i}$$

Let us consider a one-dimensional mesh to approximate $U(x)$. The nodal values can be evaluated if an accurate choice of the subdomains $S \subset \Omega$ is fulfilled. In order to carry out the finite volume discretization, a cell-centered scheme (with nodes placed in the center of the control volumes) has been chosen, as represented in the next figure

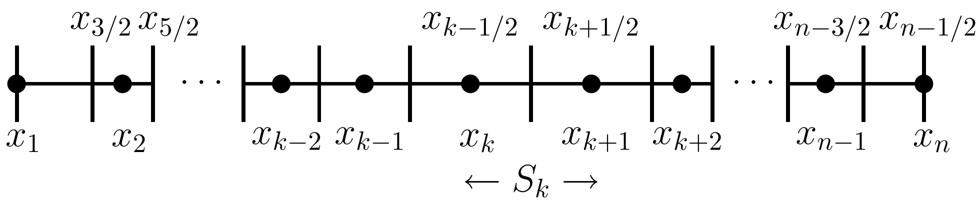

Figure 1. Finite volume discretization

The nodal coordinates are denoted by $x_1, x_2, \ldots, x_k, \ldots, x_{n-1}, x_n$ while volume coordinates are represented by $x_1, x_{3/2}, \ldots, x_{k-1/2}, x_{k+1/2}, \ldots, x_{n-1/2}, x_n$. Moreover, S_k stands for the control volume associated to node k, with extremities $k-1/2$ y $k+1/2$.

According to the new notation, expression (3) must be written as:

$$\left(-K(x)\frac{d\varphi_S(x)}{dx} + v(x)\cdot\varphi_S(x)\right)_{k+1/2} - \left(-K(x)\frac{d\varphi_S(x)}{dx} + v(x)\cdot\varphi_S(x)\right)_{k-1/2} +$$

$$\int_{S_k} q(x)\cdot\varphi_S(x)\,dx = \int_{S_k} f(x)\,dx$$

In order to approximate the exact solution $U(x)$, a scheme based on linear interpolation is being applied, since the solution supplied by this sort of interpolation has stability problems in certain situations. That's why it may be considered as a suitable scheme to check how stabilization techniques work.

Therefore, a first order piecewise polynomial function is considered to approximate $U(x)$. This function will be denoted as $u(x)$, and is expressed according to Lagrange interpolation as:

$$U(x) \cong u(x) = \sum_{k=0}^{n} u_k \cdot \phi_k(x)$$

where the $\phi_k(x)$ are the classical first order Lagrange basis functions, and u_k are the nodal values of the approached solution $u(x)$.

The first spatial derivative of the unknown $U(x)$, appearing in the dispersive-diffusive term, is calculated as:

$$\frac{\partial U(x)}{\partial x} \cong \frac{\partial u(x)}{\partial x} = \sum_{k=1}^{n} u_k \cdot \frac{d\phi_k(x)}{dx}$$

The application of this scheme leads to a system of linear equations as:

$$\mathbf{A}\cdot\times = \mathbf{b}$$

where the matrix coefficients matrix A is tridiagonal, so the system is easy to solve.

3 Stabilization technique

As it was indicated above, the linear interpolation used, entails loss of stability in certain situations, for instance when Peclet number is high. In other words, when the convective term is much bigger than the diffusive one.

One stabilization techniques is based upon the addition of some sort of artificial diffusion to the convective term.

So, considering higher order terms in Taylor expansions for the diffusive, convective, reactive and source terms (see OÑATE [1] and [2] for more details) the equation (1) may be modified as follows:

$$r - \frac{h}{2} \cdot \frac{dr}{dx} = 0 \tag{4}$$

where r is the residual given by the expression:

$$r = f(x) - \frac{d}{dx}\left(v(x) \cdot U(x) - K(x)\frac{dU(x)}{dx}\right) - q(x) \cdot U(x)$$

and h is the so called, "characteristic length".

This stabilization technique consists of evaluating the optimal value of the "characteristic length" over each element $h^{(e)}$, in order to obtain a stable solution. With this purpose, the following procedure may be used (described in OÑATE [1] and [2]):

Suppose an approached solution, $u(x)$, of the problem (4) has been achieved, by means of a numerical scheme (for example, a finite volume one). When the $u(x)$ es replaced in (4), it can be rewritten as:

$$\hat{r} - \frac{h}{2} \cdot \frac{d\hat{r}}{dx} = r \tag{5}$$

where

$$\hat{r} = f(x) - \frac{d}{dx}\left(v(x) \cdot u(x) - K(x)\frac{du(x)}{dx}\right) - q(x) \cdot u(x)$$

In expression (5), r represents the residual.

Denoting by the super-index (e) the restriction of equation (5) to each element, the following expression will be obtained:

$$\hat{r}^{(e)} - \frac{h^{(e)}}{2} \cdot \frac{d\hat{r}^{(e)}}{dx} = r^{(e)} \tag{6}$$

where: $e = 1, \ldots, NE$, being NE the number of elements ($NE = n - 1$).

Let us suppose that, using the same partition of the interval as before, an improved residual has been achieved. This may be fulfilled, for instance, smoothing derivatives (see OÑATE [1] y [2]). Denoting by $r_1^{(e)}$ and $r_2^{(e)}$ the elementary residuals due to the first solution and the improved one, respectively, it will happen:

$$r_1^{(e)} - r_2^{(e)} \tag{7}$$

Taking into account expressions (5) and (6), it is easily obtained:

$$h^{(e)} \geq 2\frac{\hat{r}_2^{(e)} - \hat{r}_1^{(e)}}{\frac{d\hat{r}_2^{(e)}}{dx} - \frac{d\hat{r}_1^{(e)}}{dx}} \tag{8}$$

Let introduce a so-called stabilization parameter, $\tilde{\alpha}^{(e)}$, defined as: $\tilde{\alpha}^{(e)} = \frac{h^{(e)}}{l^{(e)}}$ where $l^{(e)}$ is a characteristic dimension of the element (in 1-D problems, it is usually the element length: $l^{(e)} = x_{k+1} - x_k$). So, taking into account the expression (8), the stabilization parameter will adopt the form:

$$\tilde{\alpha}^{(e)} \geq \frac{2}{x_{k+1} - x_k} \cdot \frac{\hat{r}_2^{(e)} - \hat{r}_1^{(e)}}{\frac{d\hat{r}_2^{(e)}}{dx} - \frac{d\hat{r}_1^{(e)}}{dx}} \tag{9}$$

The stabilization parameter is given an initial value in between 0 and 1, and is fitted, according to the following iterative process (see OÑATE [1] and [2]):

1) Solve the stabilized problem by the finite volume scheme to obtain nodal values: u_k
2) Obtain a residual by a simple approach of the derivatives, using the nodal values achieved in step 1); $\hat{r}_1^{(e)}$
3) Obtain another residual by a smoother approximation of the derivatives: $\tilde{r}_2^{(e)}$
4) Evaluate the stabilization parameters, $h^{(e)}$ and $\tilde{\alpha}^{(e)}$, using the expressions (8) and (9)
5) Repeat the process is finished, a stable solution is obtained.

When this iterative process is finished, a stable solution is obtained.

4 Numerical results

Let us consider the boundary problem:

$$\frac{d}{dx}[(1000x + 2)U] - \frac{d}{dx}\left(2x \cdot \frac{dU}{dx}\right) - 1000 \cdot U = 0$$

$$0 \leq x \leq 5, \quad U(0) = 1, \quad U(5) = 0$$

The analytical solution is given by

$$U(x) = \frac{e^{50000 - e^{500x}}}{e^{50000} - 1}$$

which is represented in Figure 2:

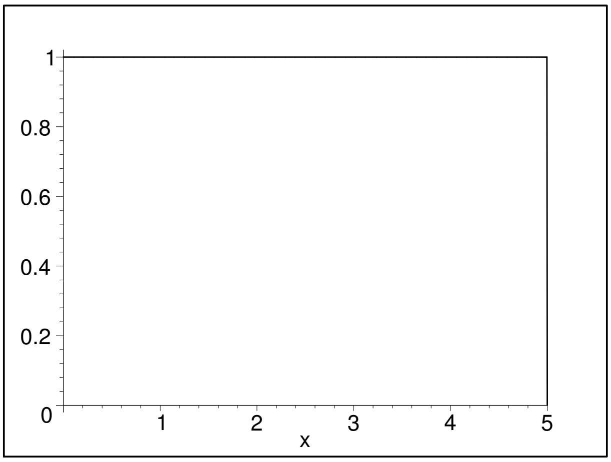

Figure 2. Analytical solution

Figure 3 shows the numerical solution obtained by the finite volume method, with linear interpolation, described before, while Figure 4 shows the numerical solution after the stabilization process

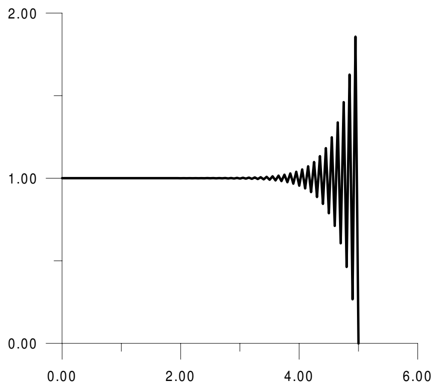

Figure 3. Non-stabilized solution

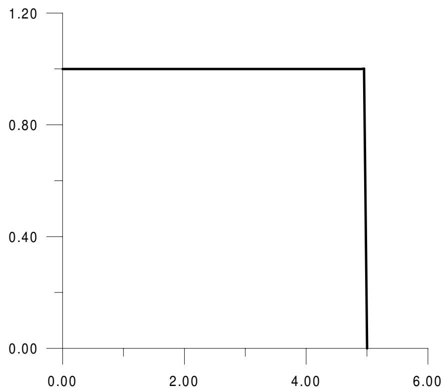

Figure 4. Stabilized solution

5 Conclusions and future research

This stabilization technique works quite well in stationary problems, even with space-depending physical parameters.

Some work is being done for its application to time depending problems, bidimensional problems and Neumann boundary conditions. An extension to time depending problems may be found in Oñate and Manzan [3].

Comparison to other stabilization techniques (ENO schemes, upwinding,...) are also being carried out.

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