A box scheme for convection-diffusion equations

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ABSTRACT. *In this paper, we describe a box-scheme for convection-diffusion equations, which is accurate both in the stationary and unstationary regimes and working in the whole range of Peclet numbers, from pure diffusion ($Pe = 0$) to pure convection ($Pe = +\infty$). The principle of the design is described for the onedimensional case, and we extend it to multidimensions by an ADI technique. Some numerical results are presented. The underlying application is the numerical simulation of the convection-diffusion of contaminants in porous media, when sharp contrasts of the diffusion coefficients occur.*

KEYWORDS: *Box scheme, finite volume method, ADI method, convection-diffusion equation, porous media, contaminants transport*

1. Introduction

In this paper, we introduce a box scheme for the unstationary convection-diffusion equation, following principles previously introduced by B. Courbet in [COU 90] for hyperbolic problems. The underlying motivation is to design a conservative numerical method well suited for convection-diffusion problems where sharp contrasts in the diffusion occur. This is the case for instance in contaminants transport problems in hydrogeology. Classicaly, the elliptic equation for the velocity (Darcy law) is solved by a mixed finite element method. The contaminants convection-diffusion equations are solved by upwind methods like finite volumes or discontinuous Galerkin. In such methods, the amount of artificial diffusion is not controlled. One of the interest of the box scheme is that one can control explicitely the amount of numerical viscosity present in the convection-diffusion equation. In addition, the formulation is of mixed type, and the diffusive flux is reconstructed in function of the primary unknown by a local formula. The scheme is relevant for Peclet numbers ranging from

0 (pure diffusion) to $+\infty$ (pure convection). After presenting the scheme in 1D, we extend it in 2D by an ADI like technique. Finally we present some preliminary numerical results on simple test cases in 1D and 2D.

2. The box scheme for the 1D problem

2.1. *Design of the scheme*

We consider the linear unstationary convection-diffusion equation with constant coefficients in the segment $I =]0,1[$.

$$\begin{cases} u_t + cu_x - \varepsilon u_{xx} = f(x)\,, \qquad x \in I \\ u\,(x,0) = u_0(x)\,, \quad x \in I \\ u\,(0,t) = 0, \quad u\,(1,t) = 0 \end{cases} \tag{1}$$

Equation (1) is recasted in mixed form with unknowns $u(.,t)$ $p(.,t)$ as

$$\begin{cases} u_t + cu_x + p_x = f(x,t)\ , \ \ x \in]0;1[\ , \ c \in \mathbb{R}\ \ , \ \ \varepsilon > 0 \quad (a) \\ p = -\varepsilon u_x \qquad (b) \\ u(x,0) = u_0(x) \quad x \in]0;1[\\ u(0,t) = u(1,t) = 0\ , \quad t \in [0;T[\end{cases} \tag{2}$$

where cu is the convective flux and $p = -\varepsilon u_x$ is the diffusive flux. Suppose given a possibly irregular mesh of the interval $]0,1[$ with nodes $x_1 = 0 < x_2 < \ldots < x_N = 1$. We call $K_{j-1/2} = [x_{j-1}\ , x_j]$ a "box" for $2 \leq j \leq N$. The lenght of the box $K_{j-1/2}$ is $h_{j-1/2} = x_j - x_{j-1}$. Integrating $(2)_a$, $(2)_b$ over the box $K_{j-1/2}$ yields

$$\begin{cases} \bullet \quad h_{j-1/2}\,(\dot{\overline{\Pi^0\,u}})_{|j-1/2}\,(t) + c\,[u\,(x_j\ , t) - u\,(x_{j-1}\ , t)] \\ +[p\,(x_j\ , t) - p(x_{j-1}\ , t)] = h_{j-1/2}\,(\Pi^0\,f)_{|j-1/2}\,(t) \\ \bullet \quad h_{j-1/2}\,(\Pi^0\,p)_{|j-1/2}\,(t) = -\varepsilon\,[u\,(x_j\ , t) - u\,(x_{j-1}\ , t)] \\ \bullet \quad u\,(x_1\ , t) = u\,(x_N\ , t) = 0 \end{cases} \tag{3}$$

Π^0 is the projector onto the piecewise constant functions into the boxes. Contrary to the finite volume method, where numerical flux formulas are used, we introduce an upwinding in (3) at the level of the quadrature formula for approximating the averaged values of $(\Pi^0 u)_{j-1/2}$ and $(\Pi^0 p)_{j-1/2}$ of u and p in each box [COU 90, CRO 02a, CRO 02b]

$$\begin{cases} (\Pi^0 u)_{j-1/2} \simeq \bar{u}_{j-1/2} = (u_j + u_{j-1})/2 + D_{u,j-1/2}(u_j - u_{j-1}) \\ (\Pi^0 p)_{j-1/2} \simeq \bar{p}_{j-1/2} = (p_j + p_{j-1})/2 - D_{p,j-1/2}(p_j - p_{j-1}) \end{cases} \tag{4}$$

$D_{u,j-1/2}$ and $D_{p,j-1/2}$ are upwinding coefficients taking different values in each box $K_{j-1/2}$. After identification of $p_j(t)$ between the two boxes $K_{j-1/2}$, $K_{j+1/2}$, we obtain a semi-discrete problem with N unknows $u_j(t)$, and an explicit reconstruction formula for $p_j(t)$.

$$
\begin{cases}
\bullet \quad h_{j+1/2}(\frac{1}{2} - D_{p,j+1/2})\dot{u}_{j+1/2}(t) + h_{j-1/2}(\frac{1}{2} + D_{p,j-1/2})\dot{u}_{j-1/2}(t) \\
= -[(\frac{1}{2} - D_{p,j+1/2})c - \frac{\varepsilon}{h_{j+1/2}}](u_{j+1}(t) - u_j(t)) \\
-[(\frac{1}{2} + D_{p,j-1/2})c + \frac{\varepsilon}{h_{j-1/2}}](u_j(t) - u_{j-1}(t)) \\
+h_{j+1/2}(\frac{1}{2} - D_{p,j+1/2})\,\Pi^0 f_{|j-1/2}(t) + h_{j-1/2}(\frac{1}{2} + D_{p,j-1/2})\,\Pi^0 f_{|j-1/2}(t) \\
\bullet \quad p_{j-1}(t) = h_{j-1/2}[\frac{1}{2} - D_{p,j-1/2}]\dot{u}_{j-1/2}(t) \\
+h_{j-1/2}[(\frac{1}{2} - D_{p,j-1/2})\frac{c}{h_{j-1/2}} - \frac{\varepsilon}{h^2_{j-1/2}}](u_j(t) - u_{j-1}(t)) \\
-h_{j-1/2}(\frac{1}{2} - D_{p,j-1/2})(\Pi^0 f)_{|j-1/2}(t) \\
\bullet \quad p_j(t) = h_{j-1/2}[-\frac{1}{2} + D_{p,j-1/2}]\dot{u}_{j-1/2}(t) \\
-h_{j-1/2}[(\frac{1}{2} + D_{p,j-1/2})\frac{c}{h_{j-1/2}} + \frac{\varepsilon}{h^2_{j-1/2}}](u_j(t) - u_{j-1}(t)) \\
+h_{j-1/2}(\frac{1}{2} + D_{p,j-1/2})\Pi^0 f_{|j-1/2}(t) \\
\bullet \quad u_1(t) = u_N(t) = 0
\end{cases}
$$

After time-integration by a θ-scheme, the scheme results in a 3-point implicit compact scheme for the unknown u, which reads

$$
(B - k\theta C)u^{n+1} = (B + k(1-\theta)C)u^n \tag{5}
$$

where B, C are the tridiagonal operators defined by :

$$
\begin{cases}
\bullet \quad Bv = [h_{j+1/2}(\frac{1}{2} - D_{p,j+1/2})(\frac{1}{2} + D_{u,j+1/2})]v_{j+1} \\
+[h_{j+1/2}(\frac{1}{2} - D_{p,j+1/2})(\frac{1}{2} - D_{u,j+1/2}) + h_{j-1/2}(\frac{1}{2} + D_{p,j-1/2})(\frac{1}{2} + D_{u,j-1/2})]v_j \\
+[h_{j-1/2}(\frac{1}{2} + D_{p,j-1/2})(\frac{1}{2} - D_{u,j-1/2})]v_{j-1} \\
\bullet \quad Cv = [-(\frac{1}{2} - D_{p,j+1/2})c + \frac{\varepsilon}{h_{j+1/2}}]v_{j+1} \\
+[(\frac{1}{2} - D_{p,j+1/2})c - \frac{\varepsilon}{h_{j+1/2}} - (\frac{1}{2} + D_{p,j-1/2})c - \frac{\varepsilon}{h_{j-1/2}}]v_j \\
+[(\frac{1}{2} + D_{p,j-1/2})c + \frac{\varepsilon}{h_{j-1/2}}]v_{j-1}
\end{cases}
$$

In addition, a reconstruction for the diffusive flux p^{n+1} is available in function of p^n, u^n, u^{n+1}.

2.2. *Stability, Accuracy*

In the particular case of a equally spaced mesh (and with $f = 0$), we perform a finite difference analysis with respect to stability and accuracy.

Proposition 1 : *(***Stability)**
Let $\tilde{D}_u = D_u + \lambda(\theta - \frac{1}{2})$.
The scheme is stable in the Von Neumann sense if and only if
(i) $\tilde{D}_u\lambda + \mu \geq 0$
(ii) $(D_p\lambda + \mu)(\tilde{D}_u D_p + (\theta - \frac{1}{2})\mu) \geq 0$
where $\lambda = ck/h$, $\mu = \varepsilon k/h^2$.

Proposition 2 *: (***Accuracy)**
The equivalent equation of scheme (5), which describes the dissipative and dispersive properties, is:

$$u_t + cu_x - \varepsilon u_x = hE_2 u_{xx} + h^2 E_3 u_{xxx} + O(h^3) \tag{6}$$

where

$$E_2 = c\tilde{D}_u \ \textit{and}\ E_3 = c[\frac{1}{12}(1-\lambda^2) - \tilde{D}_u^2] - \frac{\varepsilon}{h}[\tilde{D}u + (\theta - \frac{1}{2})\lambda - D_p] \tag{7}$$

The upwinding parameter D_u plays a role only in the transient, whereas the parameter D_p plays a role both at the stationary state and in the transient. In practice we select D_p in order to have no oscillating mode at the stationary state by, [CRO 02a] (we note the Peclet number $\mathrm{Pe} = |c|h/2\varepsilon$)

$$D_p = \frac{1}{2}\,\mathrm{sgn}(c)\max(0, 1 - \frac{1}{\mathrm{Pe}}) \tag{8}$$

The parameter D_u is selected in order to tune the amount of artificial dissipation, according to (7). Note that the dispersive coefficient is now given by (7). In practice, we choose $D_u = \frac{1}{2}\,\mathrm{sgn}(c)\max(0, \frac{1}{\mathrm{Pe}_0} - \frac{1}{\mathrm{Pe}})$, with $\mathrm{Pe}_0 \geq 1$ is some threshold Peclet number. We have taken $\mathrm{Pe}_0 = 2.5$ in the numerical tests.

2.3. *Numerical results*

Let us consider the following 1D convection-diffusion equation, where sharp contrasts in $\varepsilon(x)$ (up to 10^6) occur

$$\begin{cases} u_t + cu_x - (\varepsilon(x)u_x)_x = 0 \qquad x \in]0,1[\\ u\,(x,0) = u_0(x), \quad x \in]0,1[\\ u\,(0,t) = 1, \quad u\,(1,t) = 0 \end{cases} \tag{9}$$

where

$$\varepsilon(x) = 10^{-6}\chi_{]0;0.15[} + \chi_{]0.15;0.25[} + 10^{-3}\chi_{]0.25;0.35[} + 10^{-1}\chi_{]0.35;0.45[} + \chi_{]0.45;1[}$$

We display on Fig. 1-6 the values of $u(x,t)$, $p(x,t) = -\varepsilon u_x$ at times $T_1 = 0.084$, $T_2 = 0.175$, $T_3 = 0.238$, $T_4 = 0.350$, $T_5 = 0.525$, $T_6 = 1.519$. The maximum CFL number is $|\lambda| = 0.7$, and the Crank-Nicholson parameter $\theta = 0.5$ is used. We have 101 points (100 boxes). The parameters $D_{u,j-1/2}$, $D_{p,j-1/2}$ are selected independently in each box according to the preceding remarks.

3. Extension in 2D by the ADI method

A possible extension to the 2D equation $u_t + c.\nabla u - \varepsilon\Delta u = f(x,y,t)$ can be obtained on a regular finite difference mesh, by a ADI-like method. If A_x and

A_y are respectively the linear box operators associated to the onedimensional unstationary convection-diffusion problem in x and y direction, the $2D$ scheme is in the homogeneous case ($f = 0$):

$$(I - k\theta A_x)(I - k\theta A_y)u^{n+1} = (I + k(1-\theta)A_x)(I + k(1-\theta)A_y)u^n \qquad (10)$$

We solve this problem by the Peaceman and Rachford factorised algorithm :

$$\begin{cases} (I - k\theta A_x)u^{n+1/2} = (I + k(1-\theta)A_y)u^n \\ (I - k\theta A_y)u^{n+1} = (I + k(1-\theta)A_x)u^{n+1/2} \end{cases} \qquad (11)$$

Here we have $A_x = B_x^{-1}C_x$, $A_y = B_y^{-1}C_y$, where B_x, C_x, B_y, C_y are the 1D horizontal and vertical operators defined by (5).
To compute u^{n+1}, we solve successively the following linear systems with unknows $u_1, u^{n+1/2}, u_2, u^{n+1}$:
1) $B_y u_1 = (B_y + k(1-\theta)Cy)u^n$
2) $(B_x - k\theta C_x)u^{n+1/2} = B_x u_1$,
3) $B_x u_2 = (B_x + k(1-\theta)Cx)u^{n+1/2}$
4) $(B_y - k\theta Cy)u^{n+1} = B_y u_2$.
As an example, we have performed the test proposed in [NOY 89, TRU 01], which consists of the convection-diffusion of a $2D$ Gaussian pulse by the equation $u_t + c\nabla u - \varepsilon\Delta u = 0$ along the diagonal of the square $\Omega =]0;2[^2$ from $(x_0, y_0) = (0.5, 0.5)$ to $(x_f, y_f) = (1.5, 1.5)$. The exact solution, specified on the boundary, is:

$$g(x,y,t) = (\frac{1}{4t+1})\exp[-\frac{(x - c_1 t - x_0)^2}{\varepsilon(4t+1)} - \frac{(y - c_2 t - y_0)^2}{\varepsilon(4t+1)}] \qquad (12)$$

where $c_1 = c_2 = 0.8$ and $\varepsilon = 0.01$. The numerical solution is computed at final time $t_f = 1.25$ with $\theta = 0.5$ on the two following meshes:
- a coarse mesh made up of 4096 nodes (64 points on x-axis and 64 points on y-axis)
- a fine mesh made up of 10201 nodes (101 points on x-axis and 101 points on y-axis).
The numerical results are presented in the following table, in comparison with the ones obtained in [TRU 01] by a second order control volume method with flux limiting, on the same mesh.

Mesh size	coarse$_{box}$	fine$_{box}$	coarse$_{TT}$	fine$_{TT}$
Peak height	0.1636	0.1660	0.1382	0.1518
e_{TT}	1.0844e-5	9.4819e-7	4.9754e-5	1.4245e-5

In order to compare the computed solution with the exact one, we use the height of the Gaussian pulse $g(1.5, 1.5, 1.25) = 1/6 \simeq 0.1667$ and the mesh dependent error used in [TRU 01]

$$e_{TT} = \frac{1}{n_x n_y}\sqrt{\frac{\sum_{i=1}^{n_x}\sum_{j=1}^{n_y}(u(i,j) - g(x(i), y(j), t_0))^2}{\sum_{i=1}^{n_x}\sum_{j=1}^{n_y}u(i,j)^2}} \qquad (13)$$

where n_x and n_y are the number of points in the x and y directions.

4. Conclusion

The introduced box-scheme is a conservative method. It works on an irregular 1D finite-element mesh. It can be seen as a natural generalization to an irregular mesh of the finite difference so called "compact" schemes, or of Keller's box scheme, [KEL 71]. The ADI extension presented here is performed only for convenience, not for design reasons. We intend to explore a possible extension of the principles presented here to 2D unstructured meshes, using the method introduced in [COU 98, CRO 00] for elliptic problems, the aim being to provide alternative schemes to the finite-volume methods with numerical fluxes, which are difficult to design for diffusive problems.

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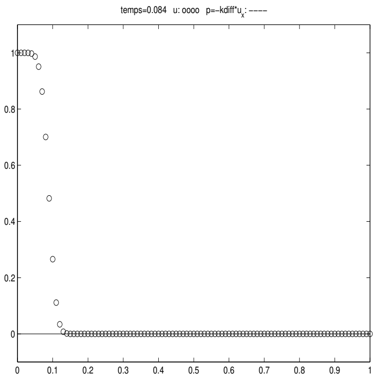

Figure 1. *T1=0.084*

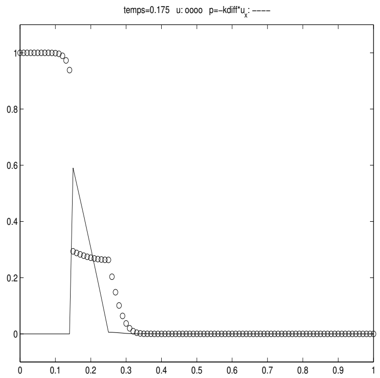

Figure 2. *T2=0.175*

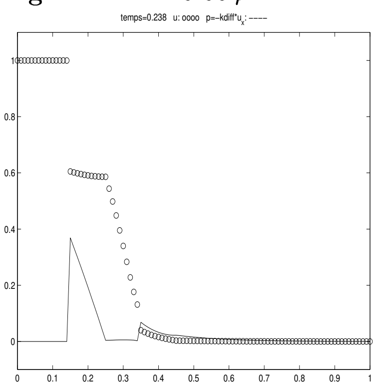

Figure 3. *T3=0.238*

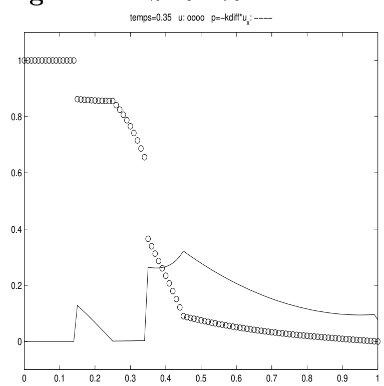

Figure 4. *T4=0.350*

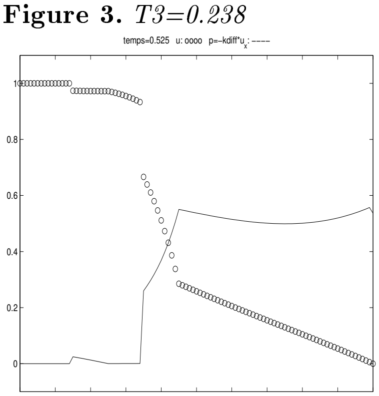

Figure 5. *T5=0.525*

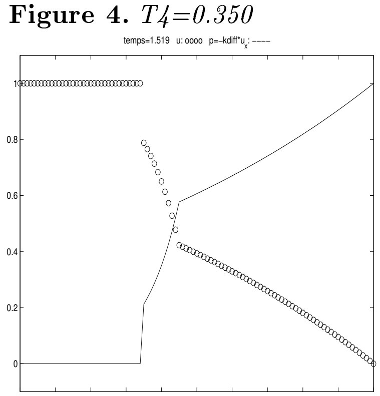

Figure 6. *T6=1.519*

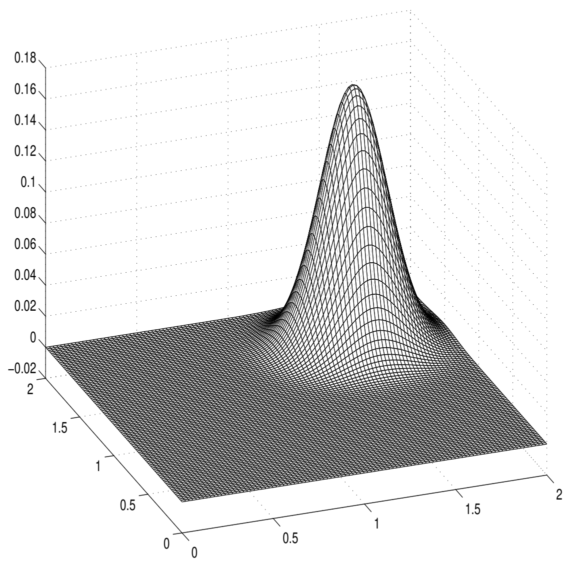

Figure 7. *The Gaussian pulse at final time* $t_f = 1.25$ *for the fine mesh.*

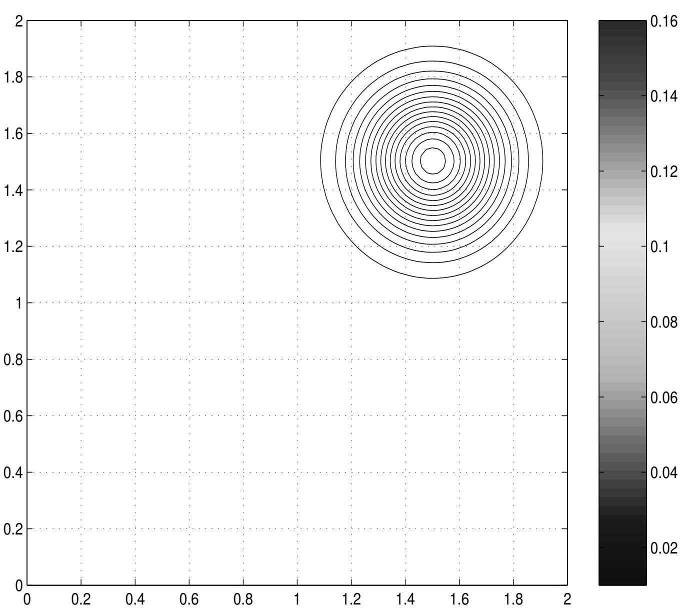

Figure 8. *Contour plots of the computed solution at final time* $t_f = 1.25$ *for the fine mesh.*