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FLOW-ORIENTED DIFFERENCE SCHEME FOR MULTIDIMENSIONAL CONVECTION-DIFFUSION EQUATION

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Abstract. In this paper one flow-oriented difference scheme for multidimensional convection-diffusion equation is constructed and analysed. The order of the accuracy is $O(\Delta x^2)$, except for convection dominant case when it decreased by one. The stability depends on the diffusion coefficient D, and for the square grid the stability condition is $D\,\Delta t/\Delta x^2 \leq 0.25$. Some examples are presented to illustrate that the scheme is especially applicable for dominantly convection problems and problems with not enough smooth solutions.

1. Introduction

The convection-diffusion equation is one of the fundamental equations of microelectronics. In the last several years there has been considerable effort aimed at semiconductor device modelling ([1],[2]). Standard finite-difference or finite element methods give rather poor results in modelling such problems, especially when the convection term is dominant, because spurious oscillations appear. The equation is officially parabolic, but practically hiperbolic as the diffusion term is negligible in comparison with the convection one. Thus, interior and boundary layers, i.e. thin regions of fast variation of the solution, appear. This causes difficulties which can hardly be surpassed by standard techniques. In [3] the necessary criteria which a good numerical discretization scheme for the convection-diffusion equation must satisfy are identified. Various ideas were implemented to develop stable and accurate methods for solving these problems ([3]-[6]).

In this paper one flow-oriented difference scheme for multidimensional convection-diffusion equation is constructed and analysed (similar approach can be found in [7]). The basic idea is given in Section 2 and it is applied and analysed for multidimensional problem in Section 3. The order of the accuracy is $O(\Delta x^2)$, except for convection dominant case when it decreased by one. The stability criterion is derived in Section 4. In the last section some examples are presented to illustrate that the scheme is especially applicable for dominantly convection problems and problems with not enough smooth solutions.

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2. Onedimensional problem

Let us begin with the onedimensional problem

$$\frac{d}{dx}(D\frac{du}{dx} - Cu) = R, \qquad x \in (0,1), \tag{1}$$

D, C and R generally depends on x and u, with arbitrary boundary conditions. The problem (1) is discretised on the uniform grid

$$\omega_x = \{x_i \,|\, x_i = i\Delta x, \Delta x = \frac{1}{n}, i = 0, \ldots, n\}.$$

By use of notation

$$V_{i+\frac{1}{2}} = (D\,\frac{dv}{dx} - C\,v)\Big|_{x=x_{i+\frac{1}{2}}}, \tag{2}$$

where $v(x)$ is the approximate solution of (1), and

$$\delta_x f(x) = \frac{1}{\Delta x}\left(f(x+\frac{\Delta x}{2}) + f(x-\frac{\Delta x}{2})\right),$$

the conservative difference approximation of the equation (1) in the interior node x_i is

$$\delta_x V_i = R(x_i, v(x_i)). \tag{3}$$

If the coefficients D and C of the equation (1) are approximated part by part by constants,

$$D(x) \equiv D_{i+\frac{1}{2}} = D(x_{i+\frac{1}{2}}, u(x_{i+\frac{1}{2}})), \quad C(x) \equiv C_{i+\frac{1}{2}} = C(x_{i+\frac{1}{2}}, u(x_{i+\frac{1}{2}})),$$

$x \in (x_i, x_{i+1})$, the relation (2) for $x \in (x_i, x_{i+1})$ can be treated as the first-order differential equation with constant coefficients, and its solution is

$$v(x) = \exp\left(\frac{C_{i+\frac{1}{2}}}{D_{i+\frac{1}{2}}}(x - x_{i+\frac{1}{2}})\right) \times \left(v(x_{i+\frac{1}{2}}) + \frac{V_{i+\frac{1}{2}}}{C_{i+\frac{1}{2}}} - \frac{V_{i+\frac{1}{2}}}{C_{i+\frac{1}{2}}}\exp\left(-\frac{C_{i+\frac{1}{2}}}{D_{i+\frac{1}{2}}}(x - x_{i+\frac{1}{2}})\right)\right). \tag{4}$$

By eliminating $v(x_{i+\frac{1}{2}})$ from (4) by use of $v(x_i)$ and $v(x_{i+1})$ we can express the term which we need for the difference approximation (3)

$$V_{i+\frac{1}{2}} = -\frac{2}{\Delta x}D_{i+\frac{1}{2}}\alpha_{i+\frac{1}{2}}\frac{v_{i+1}\exp(-\alpha_{i+\frac{1}{2}}) - v_i\exp(\alpha_{i+\frac{1}{2}})}{\exp(-\alpha_{i+\frac{1}{2}}) - \exp(\alpha_{i+\frac{1}{2}})}. \tag{5}$$

Here, $v_i = v(x_i)$ and $\alpha_{i+\frac{1}{2}} = \Delta x\, C_{i+\frac{1}{2}}/(2\,D_{i+\frac{1}{2}})$ is the mesh Peclet number, which controls the rate of mixing on the grid element. Thus from (5) and (3) the conservative difference scheme for the equation (1) becomes

$$\frac{D_{i+\frac{1}{2}}}{\Delta x^2}\left(\alpha_{i+\frac{1}{2}}\operatorname{cth}(\alpha_{i+\frac{1}{2}})(v_{i+1} - v_i) - \alpha_{i-\frac{1}{2}}\operatorname{cth}(\alpha_{i-\frac{1}{2}})(v_i - v_{i-1})\right) - \frac{1}{2\Delta x}\left(C_{i+\frac{1}{2}}(v_{i+1} + v_i) - C_{i-\frac{1}{2}}(v_i + v_{i-1})\right) = R_i. \tag{6}$$

If the coefficients D and C are constant and $R \equiv 0$, the solution of the difference equation (6) $v_i = A + B\exp(i\Delta x\, C/D)$ (A and B are appropriate constants) agreeds in the grid nodes with the solution of the equation (1) $u(x) = A + B\exp(x\, C/D)$.

For the constant coefficients central difference scheme

$$\delta_x(D\delta_x v - C\,\mu_x v)|_{x=x_i} = 0, \tag{7}$$

where $\mu_x v(x) = \frac{1}{2}\left(v(x+\frac{\Delta x}{2}) + v(x-\frac{\Delta x}{2})\right)$, the solution is

$$v_i = A + B\left(1 + \frac{\Delta x}{2}\frac{C}{D}\right)^i \left(1 - \frac{\Delta x}{2}\frac{C}{D}\right)^{-i}.$$

Thus, it is obvious that for singularly perturbed problems (small D) the solution is unstable if the mesh size is not small enough.

The expression (5) can be rewritten as

$$V_{i+\frac{1}{2}} = (D\,\delta_x v + D_\alpha\,\delta_x v - C\,\mu_x v)\Big|_{x=\frac{1}{2}(x_i+x_{i+1})}, \tag{8}$$

where $D_\alpha = D(\alpha_{i+\frac{1}{2}}\operatorname{cth}(\alpha_{i+\frac{1}{2}}) - 1)$. By comparison of the schemes (7) and (3),(8), it is obvious that the diffusion correction $D_\alpha\,\delta_x v$ made the second scheme stable also for the large Peclet number α, i.e. when the convection is dominant.

3. Multidimensional problem

Now, consider the multidimensional convection-diffusion equation. Direct implementation of the scheme (6) to every coordinate direction do not give satisfactory results, as a nonphysical diffusion in the direction normal to the convection, so called "crosswind" diffusion, produces spurious oscillations. One stable and nondissipative scheme is obtained by use in the convection direction the diffusion correction described in the previous section.

Without lose of generality, we shall treat the twodimensional problem

$$Lu \equiv \frac{\partial}{\partial x}\left(D\frac{\partial u}{\partial x} - C_x u\right) + \frac{\partial}{\partial y}\left(D\frac{\partial u}{\partial y} - C_y u\right) = R \tag{9}$$

subject to boundary conditions, on the unit square. We construct the difference scheme for the equation (9) on the rectangular grid

$$\omega_{xy} = \{(x_i, y_j)\,|\,x_i = i\Delta x, y_j = j\Delta y, \Delta x = \frac{1}{n}, \Delta y = \frac{1}{m}, i = 0,\ldots,n, j = 0,\ldots,m\},$$

To obtain the diffusion correction to the convection direction we rotate the coordinate system (x, y) for the angle

$$\theta = \operatorname{arctg}\left(C_y(x_i, y_j, u(x_i, y_j))/C_x(x_i, y_j, u(x_i, y_j))\right),$$

$$\begin{bmatrix}\xi\\ \eta\end{bmatrix} = \begin{bmatrix}\cos\theta & \sin\theta\\ -\sin\theta & \cos\theta\end{bmatrix}\begin{bmatrix}x\\ y\end{bmatrix}, \tag{10}$$

for every grid node (i,j) locally. In new coordinates, assuming that the coefficients of the equation are constant, the equation (9) is

$$D\left(\frac{\partial^2 u}{\partial \xi^2}+\frac{\partial^2 u}{\partial \eta^2}\right)-\frac{\partial}{\partial \xi}(Cu)=R, \quad (11)$$

where

$$C=\sqrt{C_x^2+C_y^2}\,\operatorname{sign}(C_xC_y).$$

To apply the approximation (6) we shall rewrite (11) as

$$D\left(\frac{\partial^2 u}{\partial \xi^2}+\frac{\partial^2 u}{\partial \eta^2}\right)-D\frac{\partial^2 u}{\partial \xi^2}+\frac{\partial}{\partial \xi}\left(D\frac{\partial u}{\partial \xi}-Cu\right)=R. \quad (12)$$

The Laplace operator is invariant towards the rotation (10), so is

$$D\left(\frac{\partial^2 u}{\partial \xi^2}+\frac{\partial^2 u}{\partial \eta^2}\right)\equiv D\left(\frac{\partial^2 u}{\partial x^2}+\frac{\partial^2 u}{\partial y^2}\right)\approx D\left(\delta_x^2 v+\delta_y^2 v\right). \quad (13)$$

Only derivatives to the ξ direction appear in the remaining two terms of the left side of the equation (12), thus the second term can be approximated by the onedimensional central difference

$$D\frac{\partial^2 u}{\partial \xi^2}\approx D\delta_\xi^2 v\equiv\frac{D}{\Delta L^2}(v_D-2v_{i,j}+v_U), \quad (14)$$

and the last one by use of the appropriate form of the scheme (6). Approximate values of the solution in the points D and U (fig.1.) are determined by the bilinear interpolation from four the nearest nodes of the grid ω_{xy}:

$$\begin{aligned} v_D&=v_{i+p,j}+\frac{\Delta x}{\Delta y}(v_{i+p,j+q}-v_{i+p,j})|\operatorname{tg}\theta| \\ v_U&=v_{i-p,j}+\frac{\Delta x}{\Delta y}(v_{i-p,j-q}-v_{i-p,j})|\operatorname{tg}\theta| \qquad |\operatorname{tg}\theta|\le\frac{\Delta y}{\Delta x}, \\ \Delta L&=\Delta x\sqrt{1+\operatorname{tg}^2\theta} \end{aligned}$$

or

$$\begin{aligned} v_D&=v_{i,j+q}+\frac{\Delta y}{\Delta x}(v_{i+p,j+q}-v_{i,j+q})|\operatorname{ctg}\theta| \\ v_U&=v_{i,j-q}+\frac{\Delta y}{\Delta x}(v_{i-p,j-q}-v_{i,j-q})|\operatorname{ctg}\theta| \qquad |\operatorname{tg}\theta|>\frac{\Delta y}{\Delta x}, \\ \Delta L&=\Delta y\sqrt{1+\operatorname{ctg}^2\theta} \end{aligned}$$

where $p=\operatorname{sign}(C_x)$ and $q=\operatorname{sign}(C_y)$.

We replace (13), (14) and (6) (where we put $v_{i+1} \equiv v_D$, $v_{i-1} \equiv v_U$) into (12) and obtain the difference approximation of the eq.(11) in the interior node of the grid ω_{xy}

$$\Lambda v \equiv D\left(\delta_x^2 v + \delta_y^2 v\right) + D\left(\alpha \ \mathrm{cth}(\alpha) - 1\right)\delta_\xi^2 v - C\mu_\xi v, \tag{15}$$

where $\alpha = C\,\Delta L/(2D)$.

For constant coefficient case and smooth boundary conditions the consistency of the approximation (15) follow from the expansion

$$\begin{aligned} Lu - \Lambda u &= D\left(\frac{\Delta x}{\Delta L}\right)^2 (\alpha \ \mathrm{cth}(\alpha) - 1)\left(\frac{\partial^2 u}{\partial x^2} + 2\frac{C_y}{C_x}\frac{\partial^2 u}{\partial x \partial y} + \frac{C_y}{C_x}\frac{\Delta y}{\Delta x}\frac{\partial^2 u}{\partial y^2}\right) + O(\Delta x^2) \\ &= \mathrm{const} * \frac{\Delta x^2}{D} + O(\Delta x^2) = \begin{cases} O(\Delta x), & \text{for } D = O(\Delta x), \\ O(\Delta x^2), & \text{for } D = O(1). \end{cases} \end{aligned} \tag{16}$$

As $\alpha \ \mathrm{cth}\,\alpha - 1 = O(\alpha^2) = O((\Delta L/D)^2)$ it is clear that for singularly perturbed problems (for small D) the order of the accuracy is decreased by one.

4. Stability of the initial-value problem

We approximate the nonstationary convection-diffusion equation

$$\frac{\partial u}{\partial t} - Lu = R, \tag{17}$$

where the operator L is defined in (9), by the second-order accurate approximation (15) accomplished via the Euler forward scheme for differentiation in time

$$\delta_t v = \Lambda v + R. \tag{18}$$

We put the Fourier expansion of the discrete solution

$$v_{i,j}^n = \sum_{m_1, m_2} \zeta^n \exp(\imath(m_1\, i\,\Delta x + m_2\, j\,\Delta y)), \tag{19}$$

to the difference equation (18) and obtain that the amplifying factor is

$$\begin{aligned} \zeta =& 1 - 4\sigma\left(\frac{C_x^2}{C_x^2 + C_y^2}(\alpha \ \mathrm{cth}(\alpha) - 1)\big(K \sin^2\frac{m_1\Delta x + m_2\Delta y}{2}\right. \\ &\left. + (1-K)\sin^2\frac{m_1\Delta x}{2}\big) + \sin^2\frac{m_1\Delta x}{2} + (\frac{\Delta x}{\Delta y})^2 \sin^2\frac{m_2\Delta y}{2}\right) \\ &- \imath C_x\sqrt{\frac{\sigma\Delta t}{D}}\big(K \sin(m_1\Delta x + m_2\Delta y) + (1-K)\sin(m_1\Delta x)\big), \end{aligned}$$

where $\sigma = D\,\Delta t/\Delta x^2$ and $K = \Delta x \ \mathrm{tg}(\theta)/\Delta y$. Therefore, we can write

$$|\zeta|^2 = f_0(m_1\Delta x, m_2\Delta y) + \Delta t\, f_1(m_1\Delta x, m_2\Delta y) + \Delta t^2\, f_2(m_1\Delta x, m_2\Delta y),$$

where

$$f_0(m_1\Delta x,m_2\Delta y) = \left(1 - 4\sigma\big(\sin^2\frac{m_1\Delta x}{2} + (\frac{\Delta x}{\Delta y})^2\sin^2\frac{m_2\Delta y}{2})\right)^2,$$

$$f_1(m_1\Delta x,m_2\Delta y) = 8\frac{C_x^2}{C_x^2+C_y^2}\frac{\sigma(\alpha\ \mathrm{cth}(\alpha)-1)}{\Delta t}\left(K\ \sin^2\frac{m_1\Delta x + m_2\Delta y}{2}\right.$$
$$\left.+(1-K)\sin^2\frac{m_1\Delta x}{2}\right)\left(4\sigma\big(\sin^2\frac{m_1\Delta x}{2} + (\frac{\Delta x}{\Delta y})^2\sin^2\frac{m_2\Delta y}{2}) - 1\right)$$
$$+ C_x^2\frac{\sigma}{D}(K\ \sin(m_1\Delta x + m_2\Delta y) + (1-K)\sin(m_1\Delta x))^2,$$

$$f_2(m_1\Delta x,m_2\Delta y) = \left(4\frac{C_x^2}{C_x^2+C_y^2}\frac{\sigma(\alpha\ \mathrm{cth}(\alpha)-1)}{\Delta t}\big(K\ \sin^2\frac{m_1\Delta x + m_2\Delta y}{2}\right.$$
$$\left.+(1-K)\sin^2\frac{m_1\Delta x}{2})\right)^2.$$

$f_1(m_1\Delta x, m_2\Delta y)$ and $f_2(m_1\Delta x, m_2\Delta y)$ are bounded functions, thus the approximation (18) will be stable for $|f_0(m_1\Delta x, m_2\Delta y)| < 1$, i.e. for

$$D\Delta t \le \frac{1}{2}\frac{(\Delta x\Delta y)^2}{\Delta x^2 + \Delta y^2}, \tag{20}$$

or, for the square grid ($\Delta x = \Delta y$), for $D\frac{\Delta t}{\Delta x^2} \le \frac{1}{4}$.

The convergence of the scheme (18) follows from the Lax's equivalence theorem ([8]).

5. Numerical results

Following examples illustrate stability and accuracy of the flow-oriented scheme (FOS) for linear and also for nonlinear problems. For the comparison results calculated by use of the central finite difference scheme (CD),

$$\delta_t v_{i,j}^n = D(\delta_x^2 v_{i,j}^n + \delta_y^2 v_{i,j}^n) + C_x\,\delta_x v_{i,j}^n + C_y\,\delta_y v_{i,j}^n,$$

and the upwind scheme (UP)

$$\delta_t v_{i,j}^n = D(\delta_x^2 v_{i,j}^n + \delta_y^2 v_{i,j}^n) + \frac{C_x}{2}\left((1-p)\delta_x v_{i+\frac{1}{2},j}^n + (1+p)\delta_x v_{i-\frac{1}{2},j}^n\right)$$
$$+ \frac{C_y}{2}\left((1-q)\delta_y v_{i,j+\frac{1}{2}}^n + (1+q)\delta_y v_{i,j-\frac{1}{2}}^n\right)$$

where $p = \mathrm{sign}(C_x)$ and $q = \mathrm{sign}(C_y)$, are presented. In all examples the square grid is used.

EXAMPLE 1. The problem is defined on the unit square by the equation

$$\frac{\partial u}{\partial t} = D\left(\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2}\right) - \cos(\theta)\,\frac{\partial u}{\partial x} - \sin(\theta)\,\frac{\partial u}{\partial y}.$$

The initial conditions are $u = 1$ for $0 \le x \le 1$, $0 \le y \le (1-x)/4$, otherwise $u = 0$. The boundary conditions are defined by the initial one and do not change in time.

Calculations are done for grid parameters $\Delta x = \Delta y = 0.05$ and time step $\Delta t = 0.002$. The direction of the convection is determined by the choise of the angle θ. FOS scheme diverges for $D = 10$, that agreed with (20) ($D\,\Delta t/\Delta x^2 = 8$), and converges for small D. The results for $\theta = 45^\circ$ and $D = 10^{-3}$ obtained by use of FOS (fig.2), CD (fig.3.) and UP (fig.4.) schemes are given. The dissipation of UP scheme is obvious, while CD scheme is very unstable. The nonlinear filtering technique proposed in [9] is applied to stabilize CD scheme (fig. 5.), but the results obtained by FOS scheme are still much better.

Fig. 2. FOS scheme

Fig. 3. CD scheme

Fig. 4. UP scheme

Fig. 5. CD + filter scheme

EXAMPLE 2. The linear problem, defined on the unit square by the equation

$$\frac{\partial u}{\partial t} = D\left(\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2}\right) - w(x,t)\,\frac{\partial u}{\partial x} - w(y,t)\,\frac{\partial u}{\partial y},$$

where $w(x,t) = (0.1A + 0.5B + C)/(A + B + C)$ and $A = \exp(-0.05(x - 0.5 + 4.95t)/D)$, $B = \exp(-0.25(x-0.5+0.75t)/D)$ and $C = \exp(-0.5(x-0.375)/D)$, is solved for $t \in (0,1)$ and $D = 10^{-4}$. The initial and Dirichlet boundary conditions are determined by the true solution $u(x,y,t) = w(x,t)\,w(y,t)$.

Fig. 6. presents FOS solution of the problem for $t = 0.6$ calculated for parameters $\Delta x = \Delta y = 0.05$ and $\Delta t = 0.002$. The comparison of the numerical solution $v(x,y,t)$ for $y = 0.6$ and $t = 0.6$ obtained for various steps $\Delta x = \Delta y$ and constant ratio $\Delta t/\Delta x^2 = 0.8$ is given on fig.7. The convergence is obvious.

Fig. 6. FOS solution for $t = 0.6$ Fig. 7. FOS solution for $y = 0.6$ and $t = 0.6$

Example 3. The nonlinear problem, defined on the unit square by the equation

$$\frac{\partial u}{\partial t} = D\left(\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2}\right) - 3u\,\frac{\partial u}{\partial x} - 3(1.5 - u)\,\frac{\partial u}{\partial y},$$

is solved for $t \in (0,1)$ and $D = 3 * 10^{-4}$. The initial and Dirichlet boundary conditions are determined by the true solution

$$u(x,y,t) = \frac{1}{4}\left(3 - \frac{1}{1 + \exp(0.375(-x + y - 0.75t)/D)}\right).$$

Fig. 8. FOS solution for $t = 0.6$ Fig. 9. FOS solution for $y = 0.6$ and $t = 0.6$

Fig. 8. presents FOS solution of the problem for $t = 0.6$ calculated for parameters $\Delta x = \Delta y = 0.05$ and $\Delta t = 0.002$. The comparison of the numerical solution $v(x, y, t)$ for $y = 0.6$ and $t = 0.6$ obtained for various steps $\Delta x = \Delta y$ and constant ratio $\Delta t/\Delta x^2 = 0.8$ is given on fig. 9. The delay of the numerical solution irrespective of the mesh size, not perceptible for the linear problem (fig. 6.), is obvious for this nonlinear problem. This might be caused by the low accurate explicit difference scheme used for time differentiation.

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