A family of finite difference schemes for the convection-diffusion equation in two dimensions

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Abstract. The construction of finite difference schemes in two dimensions is more ambiguous than in one dimension. This ambiguity arises because different combinations of local nodal values are equally able to model local behaviour with the same order of accuracy. In this paper we outline an evolution operator for the two-dimensional convection-diffusion problem in an unbounded domain and use it as the source for obtaining a family of second order (Lax-Wendroff) schemes and third-order (Quickest) schemes not yet studied in the literature. Additionally we study and compare the stability of these second-order and third-order schemes using the von Neumann method.

1 Introduction

A deceptively simple balance of convection and diffusion is related to many problems in computational fluid dynamics. Despite its simplicity, this balance is very difficult to simulate without artificial effects such as increased dispersion or oscillations degrading the solution fidelity. These effects take on increased importance in two and three-dimensional flows because of difficulty in resolving all possible length scales. Great advances in simulating convection-diffusion have occurred in the last two decades and it is now possible to devise schemes of arbitrary accuracy for constant velocity convection in an unbounded domain.

In this paper we deduce a new family of second-order schemes (that we call Lax-Wendroff schemes) and third-order schemes (that we call Quickest schemes) by using an evolution operator in an unbounded domain for the two-dimensional convection-diffusion problem. The one-dimensional Lax-Wendroff scheme is due to Lax and Wendroff [1] and the Quickest scheme was introduced by Leonard [2] as an alternative to central differencing convection or to upwinding differencing convection.

The Lax-Wendroff schemes are a class of schemes which have attained considerable stature in theoretical studies of difference schemes. The essential property of the Lax-Wendroff schemes lies in the combination of time and space-centred discretisations. Their popularity is due to their second-order accuracy and simplicity, although their behaviour around discontinuities is not fully satisfactory. The Quickest scheme was first generalised in two dimensions by Davis and Moore [3] but when generalising the method they ignored some of the cross-derivatives and that reduced the temporal accuracy of the scheme. The new Quickest schemes are expected to be more accurate in time than the Quickest scheme derived by Davis and Moore [3], since we take into account the cross-derivatives.

To analyse the practical stability of the numerical schemes we use von Neumann analysis. We observe that interesting differences occur between the stability regions of the different numerical schemes. For a clear visualisation of the stability regions we plot sufficient and necessary stability conditions in a three-dimensional space, in which the coordinates involve the convective coefficients and the diffusion.

Stability of finite difference schemes has been widely described in the literature. Two important books on stability analysis of difference methods are the classical book by Richtmyer and Morton [4] and the more recent book by Gustafsson *et al* [5]. The latter concentrates its attention in the normal mode analysis. Some of the work on stability analysis for finite difference schemes for the convection-diffusion equation using the von Neumann method was done by Beckers [6] for a scheme in three dimensions, Hindmarsh *et al* [7] for a multidimensional central scheme, Kwok and Tam [8] for leap-frog-type finite difference schemes, Siemieniuch and Gladwell [9] for central and upwind schemes, Verwer and Sommeijer [10] in relation with an odd-even-line hopscotch method, and Wesseling [11] for a fourth-order central scheme.

2 Finite differences schemes

Morton and Sobey [12] have derived schemes using the exact solution of a one-dimensional convection-diffusion problem. In this section we apply the same idea by deriving the analytic solution for a two-dimensional convection-diffusion problem and using it as the source for obtaining the finite difference schemes.

Consider the convection-diffusion equation with coefficient $D > 0$:

$$\frac{\partial u}{\partial t}(x,y,t) + V\frac{\partial u}{\partial x}(x,y,t) + W\frac{\partial u}{\partial y}(x,y,t) = D\left(\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2}\right)(x,y,t) \quad (1)$$

and the initial condition

$$u(x,y,0) = u_0(x,y). \quad (2)$$

The diffusion coefficient is taken to be positive since a negative coefficient is a physical impossibility. Using a two-dimensional Fourier transform to find the solution for the problem (1),(2) we obtain:

$$u(x,y,t)=\frac{1}{\pi}\int_{-\infty}^{+\infty}\int_{-\infty}^{+\infty}u_0(x-Vt+2\sqrt{Dt}\xi,y-Wt+2\sqrt{Dt}\tau)\mathrm{e}^{-\xi^2-\tau^2}d\xi d\tau. \tag{3}$$

This is a two-dimensional evolution operator. In a manner similar, to the one-dimensional case, it defines a Green's function $G(x,y,\Delta t)$ which gives the evolution over a single time-step:

$$u(x,y,t_n+\Delta t)=\frac{1}{\pi}\int_{-\infty}^{+\infty}\int_{-\infty}^{+\infty}u(\xi,\eta,t_n)G(x-\xi,y-\eta,\Delta t)d\xi d\eta \tag{4}$$

where $G(s,p,t)=\dfrac{1}{4Dt\pi}\mathrm{e}^{-(s-Vt)^2/4Dt}\mathrm{e}^{-(p-Wt)^2/4Dt}$.

Using the evolution operator (4) and following the same procedure as in Morton and Sobey [12] for one dimension, we can now obtain finite difference schemes by interpolation on a uniform mesh. We denote by U_{jk}^n the approximations to the values $u(x_j,y_k,t_n)$ at the mesh points $(x_j,y_k)=(j\Delta x,k\Delta y),\quad j,k=0,\pm1,\pm2,\ldots$.

We use the usual operators, central, second difference, backward and forward respectively:

$$\begin{aligned}\Delta_{x0}U_{jk}&=(U_{j+1k}-U_{j-1k})/2, &\quad \delta_x^2U_{jk}&=U_{j+1k}-2U_{jk}+U_{j-1k},\\ \Delta_{x-}U_{jk}&=U_{jk}-U_{j-1k}, &\quad \Delta_{x+}U_{jk}&=U_{j+1k}-U_{jk}.\end{aligned}$$

The operators $\Delta_{y0},\delta_y^2,\Delta_{y-},\Delta_{y+}$ are defined similarly.

We choose uniform space-steps Δx and Δy and a time-step Δt. We also define the important quantities ν_x, ν_y, μ_x and μ_y, that we are using in what follows:

$$\nu_x=\frac{V\Delta t}{\Delta x},\quad \nu_y=\frac{W\Delta t}{\Delta y}\quad \mu_x=\frac{D\Delta t}{\Delta x^2},\quad \mu_y=\frac{D\Delta t}{\Delta y^2}.$$

In the next sections we derive a family of Lax-Wendroff schemes and a family of Quickest schemes in two dimensions. Firstly we derive the schemes based on a quadratic and cubic polynomial interpolation of the function $u(\xi,\eta,t_n)$ that appears in (4). Secondly we also derive schemes by using Taylor approximations of order two and three, of the same function.

The generalisation of finite difference schemes for a convection diffusion equation to multidimensions is not just the sum of the individual one-dimensional contributions, since the simple addition of individual finite differences in x and y without appropriate cross terms can lead to a basic instability.

2.1 Polynomial approximation

In this section we obtain finite difference schemes by approximating $u(x, y, t_n)$ in (4) by a local polynomial of degree K around the point (x_j, y_k), namely,

$$p_{jk}(x,y) = \sum_{r=0}^{K}\sum_{s=0}^{K} b_{rs}(x-x_j)^r(y-y_k)^s.$$

Using the exact evolution operator, the approximation U_{jk}^{n+1} is given by

$$U_{jk}^{n+1} = \sum_{r,s=0}^{K} \frac{b_{rs}}{\pi}\int_{\mathbb{R}^2} (-V\Delta t + 2\sqrt{D\Delta t}\xi)^r(-W\Delta t + 2\sqrt{D\Delta t}\tau)^s \mathrm{e}^{-\xi^2-\tau^2} d\xi d\tau.$$

If the power terms are expanded then all the integrals can be determined and we can write:

$$\begin{aligned} U_{jk}^{n+1} &= b_{00} - b_{10}V\Delta t - b_{01}W\Delta t + b_{11}VW(\Delta t)^2 + b_{20}(2D\Delta t + V^2(\Delta t)^2) \\ &\quad + b_{02}(2D\Delta t + W^2(\Delta t)^2) - b_{30}(6DV(\Delta t)^2 + V^3(\Delta t)^3) \\ &\quad - b_{03}(6DW(\Delta t)^2 + W^3(\Delta t)^3) - b_{21}W\Delta t(2D\Delta t + V^2(\Delta t)^2) \\ &\quad - b_{12}V\Delta t(2D\Delta t + W^2(\Delta t)^2) + \ldots . \end{aligned} \tag{5}$$

Within this formula we obtain second and third-order finite difference schemes by using quadratic interpolation or cubic interpolation.

If we use a quadratic interpolation we need to choose six interpolation points to determine the six coefficients $b_{00}, b_{01}, b_{10}, b_{20}, b_{11}, b_{02}$. We obtain a different method for each choice of points. Any nodal value will have eight neighbouring points so we need to choose six points from the nine points (nodal point plus eight neighbours). We choose the points, so that they form a five-point star around (x_j, y_k) and the sixth point is selected according to the direction of the velocities V and W. For instance assume that V and W are positive. We choose the sixth interpolation point to be (x_{j-1}, y_{k-1}). Then we have the formula:

$$U_{jk}^{n+1} = [1 - \nu_x\Delta_{x0} - \nu_y\Delta_{y0} + (\frac{1}{2}\nu_x^2 + \mu_x)\delta_x^2 + (\frac{1}{2}\nu_y^2 + \mu_y)\delta_y^2 + \nu_x\nu_y\Delta_{x-}\Delta_{y-}]U_{jk}^n. \tag{6}$$

We call this scheme the Polynomial Lax-Wendroff scheme.

Clearly there are three other configurations depending on various combinations of the signs of V and W. For V negative and W positive, we choose the sixth point as (x_{j+1}, y_{k-1}). If V is positive and W negative, we consider the point (x_{j-1}, y_{k+1}) and for V and W negative we choose the point (x_{j+1}, y_{k+1}). The different possibilities can give us a different coefficient b_{11}.

Next we turn to cubic interpolation. One advantage of using high-order methods is that numerical diffusion and dispersion errors are relatively smaller than in low order methods. The procedure is illustrated for two-dimensional flow with velocity V and W positive as in the previous case. We need to use ten points to carry out this interpolation. Using the ten points U_{j-2k}, U_{j-1k-1}, U_{j-1k}, U_{j-1k+1}, U_{jk-2}, U_{jk-1}, U_{jk}, U_{jk+1}, U_{j+1k-1} and U_{j+1k} to evaluate b_{rs}, $r = 0, 1, 2, 3$; $s = 0, 1, 2, 3$ we find the scheme:

$$\begin{aligned} U_{jk}^{n+1} &= U_{jk}^n - \nu_x \Delta_{x0} U_{jk}^n - \nu_y \Delta_{y0} U_{jk}^n + (\frac{1}{2}\nu_x^2 + \mu_x)\delta_x^2 U_{jk}^n + (\frac{1}{2}\nu_y^2 + \mu_y)\delta_y^2 U_{jk}^n \\ &+ \frac{1}{2}\nu_x \nu_y \Delta_{y+}\Delta_{x-} U_{jk}^n + \frac{1}{2}\nu_x \nu_y \Delta_{x+}\Delta_{y-} U_{jk}^n \\ &+ \frac{1}{6}\nu_x (1 - \nu_x^2 - 6\mu_x)\delta_x^2 \Delta_{x-} U_{jk}^n + \frac{1}{6}\nu_y (1 - \nu_y^2 - 6\mu_y)\delta_y^2 \Delta_{y-} U_{jk}^n \\ &- \nu_y (\mu_x + \frac{1}{2}\nu_x^2)\delta_x^2 \Delta_{y-} U_{jk}^n - \nu_x (\mu_y + \frac{1}{2}\nu_y^2)\delta_y^2 \Delta_{x-} U_{jk}^n. \end{aligned} \tag{7}$$

This scheme is called the Polynomial Quickest scheme. As with the Lax-Wendroff schemes, we can change the choice of the mesh points, depending on the direction of the velocities. The changes that occur in the scheme (7) according to the sign of the velocities involve changes in the coefficients $b_{11}, b_{12}, b_{21}, b_{30}$ and b_{03}.

2.2 Taylor approximation

In the previous section we considered a local polynomial interpolation of some selected points in a neighbourhood of (x_j, y_k). Since the local interpolation requires only a small number of neighbouring points, we used the flow directions to choose which neighbouring points to use. Now we use an alternative idea and approximate $u(x, y, t_n)$ by a truncated Taylor series of degree K around (x_j, y_k):

$$t_{jk}(x, y) = \sum_{r=0}^{K} \sum_{s=0}^{K} b_{rs}(x - x_j)^r (y - y_k)^s, \tag{8}$$

where $b_{rs} = \dfrac{u_{x^r y^s}}{r!s!}$. Using the evolution operator as in the previous section, depending on the order of the expansion we can obtain the numerical schemes described below.

For the second-order accurate Taylor expansion we obtain the numerical method:

$$U_{jk}^{n+1} = [1 - (\nu_x \Delta_{x0} + \nu_y \Delta_{y0}) + (\frac{1}{2}\nu_x^2 + \mu_x)\delta_x^2 + (\frac{1}{2}\nu_y^2 + \mu_y)\delta_y^2 + \nu_x \nu_y \Delta_{x0}\Delta_{y0}] U_{jk}^n. \tag{9}$$

This scheme uses a nine-point scheme and we call it the Taylor Lax-Wendroff scheme. This method can be used independently of the sign of the velocity components.

For the third-order accurate Taylor expansion, taking in consideration that V and W are positive, we use the eleven point stencil U_{j-2k}, U_{j-1k-1},

U_{j-1k} U_{j-1k+1}, U_{jk-2}, U_{jk-1}, U_{jk}, U_{jk+1} U_{j+1k-1}, U_{j+1k}, and U_{j+1k+1}. It gives the numerical method:

$$\begin{aligned}U_{jk}^{n+1} &= U_{jk}^n - \nu_x \Delta_{x0} U_{jk}^n - \nu_y \Delta_{y0} U_{jk}^n \\ &+(\frac{1}{2}\nu_x^2 + \mu_x)\delta_x^2 U_{jk}^n + (\frac{1}{2}\nu_y^2 + \mu_y)\delta_y^2 U_{jk}^n + \nu_x \nu_y \Delta_{x0}\Delta_{y0} U_{jk}^n \\ &+\frac{1}{6}\nu_x(1-\nu_x^2 - 6\mu_x)\delta_x^2 \Delta_{x-} U_{jk}^n + \frac{1}{6}\nu_y(1-\nu_y^2-6\mu_y)\delta_y^2\Delta_{y-}U_{jk}^n \\ &-\nu_y(\mu_x + \frac{1}{2}\nu_x^2)\delta_x^2\Delta_{y0}U_{jk}^n - \nu_x(\mu_y + \frac{1}{2}\nu_y^2)\delta_y^2\Delta_{x0}U_{jk}^n. \end{aligned} \tag{10}$$

Similarly to the previous schemes, we call this scheme the Taylor Quickest scheme. The choice of the mesh points, to approximate the third derivatives, depends on the directions of the velocity components and affects the values of the coefficients b_{30} and b_{03}.

In the next section we use the von Neumann method to analyse the stability region of these four numerical schemes.

3 Von Neumann stability analysis

The von Neumann analysis in two dimensions is a straightforward generalisation of the one-dimensional case. The discrete Fourier decomposition in two dimensions consists of the decomposition of the function into a Fourier series as

$$U_{jk}^n = \sum_{\xi_x,\xi_y} \kappa^n e^{i\xi_x j\Delta x} e^{i\xi_y k\Delta y},$$

where the range ξ_x, ξ_y is defined separately for each direction, as in the one-dimensional case. The amplification factor is given by κ. The products $\xi_x\Delta x$ and $\xi_y\Delta y$ are often represented as a phase angle, namely, $\theta_x = \xi_x\Delta x,\ \theta_y = \xi_y\Delta y$. To obtain a von Neumann stability condition we insert the singular component $\kappa^n e^{ij\theta_x}e^{ik\theta_y}$ into the discretised scheme. The amplification factor is said to satisfy the von Neumann condition if there is a constant K such that

$$|\kappa(\theta_x,\theta_y)| \le 1 + K\Delta t \ \ \forall\, \theta_x,\theta_y \in [0,2\pi]. \tag{11}$$

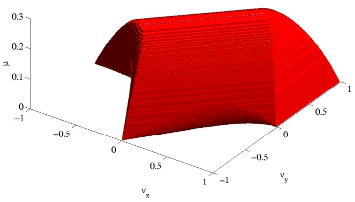
As in the one-dimensional case, in practice we use the stronger condition

$$|\kappa(\theta_x,\theta_y)| \le 1 \ \ \forall\, \theta_x,\theta_y \in [0,2\pi], \tag{12}$$

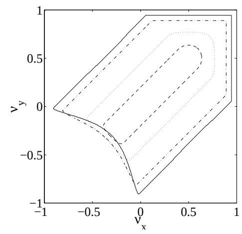
and the discrete scheme that meets this condition, we refer to as von Neumann stable. This has been called practical stability by Richtmyer and Morton [4] or strict stability by other authors. In some cases condition (11) allows numerical modes to grow exponentially in time for finite values of Δt. Therefore, the practical, or strict, stability condition (12) is recommended in order to prevent numerical modes from growing faster than the physical modes of the differential equation.

For our finite difference schemes we derive mostly analytical necessary conditions. Nevertheless we plot numerically the sufficient and necessary stability regions in the three-dimensional space (ν_x, ν_y, μ), where for simplicity we assume $\mu = \mu_x = \mu_y$.

We present below lemmas that describe only necessary stability conditions for the four numerical schemes derived in the previous section. These analytical results correspond to condition (12) for phase angles of high frequency, namely, $\theta_x = \pi$ and $\theta_y = \pi$, and for the limiting case $\theta_x \to 0, \theta_y \to 0$. Necessary and sufficient conditions for the stability of the numerical schemes are displayed in Fig. 1-4, where the stable regions are inside the surfaces.



(a)



(b)

Fig. 1. (a) von Neumann stability analysis for the Polynomial Lax-Wendroff scheme; (b) projection of the figure (a) on the plane $\nu_x \circ \nu_y$: $\mu = 0.05$ $(-)$; $\mu = 0.1$ $(-\cdot-)$; $\mu = 0.2$ $(\cdots)$; $\mu = 0.24$ $(--)$.

Lemma 1 *Necessary conditions for the Polynomial Lax-Wendroff scheme (6) to be stable are:*

$$2(\mu_x + \mu_y) \leq 1 \tag{13}$$
$$(\nu_x - \nu_y)^2 \leq 1 - 2(\mu_x + \mu_y). \tag{14}$$

Lemma 2 *Necessary conditions for the Taylor Lax-Wendroff scheme (9) to be stable are:*

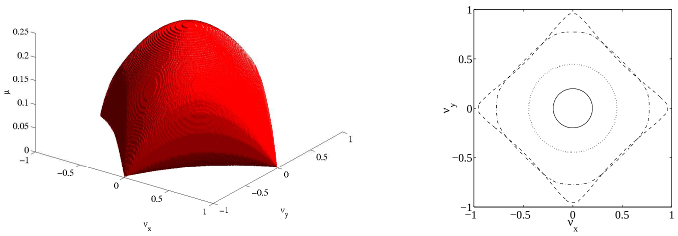
$$2(\mu_x + \mu_y) \leq 1 \tag{15}$$
$$\nu_x^2 + \nu_y^2 \leq 1 - 2(\mu_x + \mu_y). \tag{16}$$

Lemma 3 *A necessary condition for the Polynomial Quickest scheme (7) to be stable is:*

$$(\nu_x^2 + 2\mu_x)(1 - 2\nu_y) + (\nu_y^2 + 2\mu_y)(1 - 2\nu_x) + 2\nu_x\nu_y + \frac{2}{3}\nu_x(1 - \nu_x^2 - 6\mu_x) + \frac{2}{3}\nu_y(1 - \nu_y^2 - 6\mu_y) \leq 1. \tag{17}$$

Lemma 4 *A necessary condition for the Taylor Quickest scheme (10) to be stable is:*

$$(\nu_x^2 + 2\mu_x) + (\nu_y^2 + 2\mu_y) + \frac{2}{3}\nu_x(1 - \nu_x^2 - 6\mu_x) + \frac{2}{3}\nu_y(1 - \nu_y^2 - 6\mu_y) \leq 1. \quad (18)$$



(a) (b)

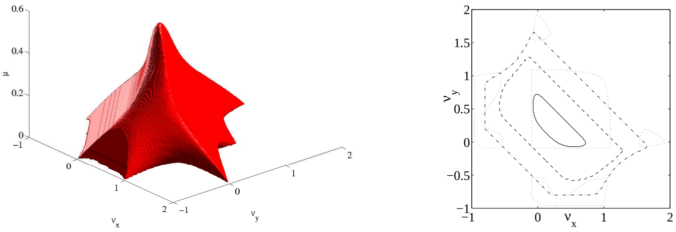
Fig. 2. (a) von Neumann stability analysis for the Taylor Lax-Wendroff scheme; (b) projection of the figure (a) on the plane $\nu_x \circ \nu_y$: $\mu = 0.02$ $(--)$; $\mu = 0.1$ $(-\cdot-)$; $\mu = 0.2$ $(\cdots)$; $\mu = 0.24$ $(-)$.

In Lemma 1 condition (14) is associated with the diagonal lines shown in Fig. 1(b), which determines the stable region to be between the two lines as we see in Fig. 1(b). Condition (13) gives us a limit for the diffusion parameter. We observe that the Polynomial Lax-Wendroff scheme is still stable for simultaneously large values of ν_x and ν_y, when μ is small. Although we plot the stability region for $(\nu_x, \nu_y) \in [-1, 1] \times [-1, 1]$, note that for this scheme we are assuming that both velocity components are positive, that is, that ν_x and ν_y are both positive.

The second lemma concerns the Taylor Lax-Wendroff scheme. Although this scheme can be used independently of the signs of the velocity components, it has a smaller region of stability for small μ, when compared with the Polynomial Lax-Wendroff scheme (6). In Fig. 2 we plot necessary and sufficient von Neumann stability conditions for the Taylor Lax-Wendroff scheme (9). In view of the Fig. 2(b), a necessary and sufficient condition for this scheme is condition (16) in Lemma 2 associated with some other condition that seems to change as μ increases from $|\nu_x|^{2/3} + |\nu_y|^{2/3} \leq 1$ to $|\nu_x| + |\nu_y| \leq 1$.

For the Polynomial Quickest scheme we have a necessary condition for the stability of the scheme in Lemma 3 and we plot sufficient and necessary conditions in figure 3. Note that on the three-dimensional surface displayed in figure 3, we have $\mu \leq 9/16$. This value corresponds to $(\nu_x, \nu_y) = (1/4, 1/4)$. The stability regions for the small μ are bigger than those of both Lax-Wendroff schemes.

Next, in Lemma 4, we provide a necessary condition for the stability of the Taylor Quickest scheme. Sufficient and necessary conditions for the



(a) (b)

Fig. 3. (a) von Neumann stability analysis for the Polynomial Quickest scheme; (b) projection of the figure (a) on the plane $\nu_x \circ \nu_y$: $\mu = 0.02$ $(\cdots)$; $\mu = 0.1$ $(-\cdot-)$; $\mu = 0.2$ $(--)$; $\mu = 0.4$ $(-)$.

Taylor Quickest scheme are shown in figure 4. By assuming $\mu_x = \mu_y = \mu$ and $\nu_x = \nu_y = 1/4$ in (18) we have the condition $\mu \leq 9/32$. This is the maximum value that μ can take inside the stable region (see figure 4).

4 Summary

In this paper we provided von Neumann stability regions for various finite difference schemes. The Lax-Wendroff schemes considered present regions of stability that are sufficient and necessary conditions, with a shape that appears to have a simple form, although we found considerable difficulties when we attempted to find these conditions analytically. The main source of these difficulties was related to the majorisation of the Fourier terms associated with the mixed derivatives. The Quickest schemes present more awkward regions and they do not seem to show an obvious regularity leading us to conjecture that to provide the analytical sufficient and necessary conditions is an extremely difficult task. Therefore we provide only the analytical necessary conditions, although sufficient and necessary regions of stability are calculated numerically. We know that the presence of boundary conditions interferes with the stability of a finite difference scheme. Although in the presence of boundaries that are not periodic the von Neumann condition is no longer a sufficient condition, it remains an important necessary condition.

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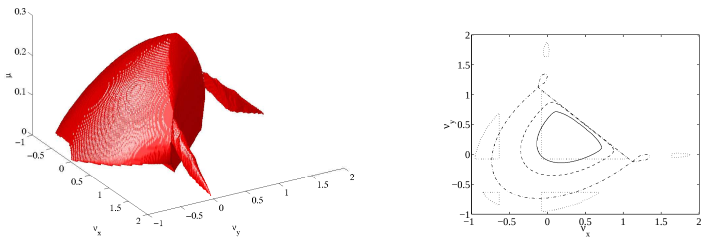

(a) (b)

Fig. 4. (a) von Neumann stability analysis for the Taylor Quickest scheme; (b) projection of the figure (a) on the plane $\nu_x \circ \nu_y$: $\mu = 0.02$ $(\cdots)$; $\mu = 0.1$ $(- \cdot -)$; $\mu = 0.2$ $(--)$; $\mu = 0.24$ $(-)$.

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