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by

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# A two-dimensional complete flux scheme in local flow adapted coordinates

Jan ten Thije Boonkkamp, Martijn Anthonissen and Ruben Kwant

**Abstract** We present a formulation of the two-dimensional complete flux (CF) scheme in terms of local orthogonal coordinates adapted to the flow, i.e., one coordinate axis is aligned with the local velocity field and the other one is perpendicular to it. This approach gives rise to an advection-diffusion-reaction boundary value problem (BVP) for the flux component in the local flow direction. For the other (diffusive) flux component we use central differences. We will demonstrate the performance of the scheme for several examples.

**Key words:** conservation laws, finite volume method, numerical flux, complete flux scheme, local orthogonal coordinates.

**MSC (2010):** 65N08, 65N99

## 1 Introduction

Conservation laws occur frequently in science and engineering, modeling a wide variety of phenomena, for example laminar flames or gas discharges in plasmas. These conservation laws are often of advection-diffusion-reaction type, describing the interplay between different processes such as advection or drift, diffusion or conduction and (chemical) reactions or impact ionization. We restrict ourselves to stationary two-dimensional conservation laws.

The prototypical conservation law reads

$$\nabla \cdot (\mathbf{u}\varphi - \varepsilon \nabla \varphi) = s, \quad (1)$$

where, for example,  $\mathbf{u} = u\mathbf{e}_x + v\mathbf{e}_y$  is a flow velocity,  $\varepsilon \geq \varepsilon_{\min} > 0$  a diffusion coefficient and  $s$  a reaction rate. The unknown  $\varphi$  might be the mass fraction of one of the constituent species in a laminar flame or a plasma. Associated with (1) we introduce the flux (vector)  $\mathbf{f} = f_x\mathbf{e}_x + f_y\mathbf{e}_y$ , given by

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$$\mathbf{f} = \mathbf{u}\varphi - \varepsilon\nabla\varphi. \quad (2)$$

Consequently, the conservation law can be concisely written as  $\nabla\cdot\mathbf{f} = s$ . Integrating this equation over a fixed domain  $\Omega$  and applying Gauss's law we obtain the integral form of the conservation law, i.e.,

$$\oint_{\partial\Omega} \mathbf{f}\cdot\mathbf{n} ds = \int_{\Omega} s dA, \quad (3)$$

where  $\mathbf{n}$  is the unit outward normal on the positively oriented boundary  $\partial\Omega$ .

For space discretization of (1) we employ the finite volume method (FVM). To that purpose, we introduce grid points  $\mathbf{x}_{i,j} = (x_i, y_j)$  where  $\varphi$  has to be approximated and control volumes  $\Omega_{i,j} = (x_{i-1/2}, x_{i+1/2}) \times (y_{j-1/2}, y_{j+1/2})$  covering the domain. Here  $x_{i\pm 1/2} = \frac{1}{2}(x_i + x_{i\pm 1})$  etc. Taking  $\Omega = \Omega_{i,j}$  in (3) and approximating all integrals involved with the midpoint rule, we find

$$\Delta y(F_{x,i+1/2,j} - F_{x,i-1/2,j}) + \Delta x(F_{y,i,j+1/2} - F_{y,i,j-1/2}) = \Delta x\Delta y s_{i,j}, \quad (4)$$

where  $F_{x,i+1/2,j}$  is the approximation of  $f_x$  at the interface point  $(x_{i+1/2}, y_j)$  etc. and  $s_{i,j} = s(\mathbf{x}_{i,j})$ . The FVM has to be completed with numerical approximations of all fluxes.

For the numerical flux approximation we employ the complete flux (CF) scheme introduced in [4]. The basic idea of this scheme is to compute the numerical flux from a local *one-dimensional* boundary value problem for the conservation law, including the source term. For one-dimensional problems the scheme gives excellent results and is proven to be uniformly second order convergent [1]. The generalization of this approach to two-dimensional problems is tedious. Instead, the one-dimensional CF scheme is often applied componentwise ignoring the cross-flux terms. For dominant diffusion this version of the scheme is still adequate, however, for dominant advection the scheme suffers from significant numerical diffusion. To remedy this problem, we have included the cross flux as an artificial source term in the local one-dimensional BVPs, virtually eliminating diffusion. This modified scheme is able to reproduce very steep layers in the solution of (1).

However, for three-dimensional conservation laws this approach is rather cumbersome and adds too much anti-diffusion. Therefore we adopt another approach which is expected to be more suitable. Inspired by the skew upstream differencing schemes introduced in [2], we define a local  $(\xi, \eta)$ -coordinate system adapted to the local velocity  $\mathbf{u}$  and compute the flux components in this coordinate system. This way, we obtain a  $\xi$ -component of the flux parallel to  $\mathbf{u}$  and an  $\eta$ -component perpendicular to  $\mathbf{u}$ , which can be combined to the normal component of the numerical flux. For both components we use a one-dimensional flux approximation scheme. For the  $\xi$ -component we take into account the full advection-diffusion-reaction balance, and include the easy to compute (diffusive) cross flux term as an additional source. On the other hand, for the  $\eta$ -component, we restrict ourselves to the homogeneous flux scheme [4]. The resulting scheme exhibits uniform second order convergence.

We have organized our paper as follows. In Section 2 we outline the one-dimensional complete flux scheme, and subsequently in Section 3, we present the two-dimensional scheme in local, flow adapted coordinates. Next, in Section 4 we demonstrate the performance of the scheme for two examples. Concluding remarks are given in Section 5.

## 2 One-dimensional complete flux scheme

In this section we outline the one-dimensional version of the complete flux scheme; for more details see [4].

The one-dimensional conservation law can be concisely written as  $df/dx = s$  with  $f = u\varphi - \varepsilon d\varphi/dx$ . The integral representation of the flux  $f_{j+1/2} = f(x_{j+1/2})$  at the cell edge  $x_{j+1/2}$  is based on the following two-point BVP:

$$\frac{df}{dx} = \frac{d}{dx} \left( u\varphi - \varepsilon \frac{d\varphi}{dx} \right) = s, \quad x_j < x < x_{j+1}, \quad (5a)$$

$$\varphi(x_j) = \varphi_j, \quad \varphi(x_{j+1}) = \varphi_{j+1}, \quad (5b)$$

consequently, the flux will be the superposition of a homogeneous flux, corresponding to the advection-diffusion operator, and an inhomogeneous flux, taking into account the effect of the source term. Let us first introduce the following variables/notation:

$$a = \frac{u}{\varepsilon}, \quad P = a\Delta x, \quad A(x) = \int_{x_{j+1/2}}^x a(z) dz, \quad \langle p, q \rangle = \int_{x_j}^{x_{j+1}} p(x)q(x) dx. \quad (6)$$

We refer to  $P$  and  $A$  as the (grid) Péclet function and integral, respectively, generalizing the well-know (grid) Péclet number. Using the integrating factor formulation of (5a) we can derive the following representation for the flux:

$$f_{j+1/2} = f_{j+1/2}^h + f_{j+1/2}^i, \quad (7a)$$

$$f_{j+1/2}^h = (e^{-A(x_j)}\varphi_j - e^{-A(x_{j+1})}\varphi_{j+1}) / \langle \varepsilon^{-1}, e^{-A} \rangle, \quad (7b)$$

$$f_{j+1/2}^i = \Delta x \int_0^1 G(\sigma) s(x(\sigma)) d\sigma, \quad (7c)$$

where  $f_{j+1/2}^h$  and  $f_{j+1/2}^i$  are the homogeneous and inhomogeneous part of the flux, respectively. In (7c) the function  $G$ , depending on the scaled coordinate  $\sigma(x) = (x - x_j)/\Delta x$ , is the so-called the Green's function for the flux, since it relates the source to the flux, different from the usual Green's function, which relates the source to the solution.

To determine the numerical flux  $F_{j+1/2}$  we restrict ourselves to constant  $u$  and  $\varepsilon$ . Moreover, we take  $s$  piecewise constant, i.e.,  $s(x) = s_j$  for  $x_{j-1/2} < x < x_{j+1/2}$ . In this case we can evaluate all integrals involved exactly and find:

$$F_{j+1/2} = F_{j+1/2}^h + F_{j+1/2}^i, \quad (8a)$$

$$F_{j+1/2}^h = \frac{\varepsilon}{\Delta x} (B(-P)\varphi_j - B(P)\varphi_{j+1}), \quad (8b)$$

$$F_{j+1/2}^i = \Delta x (C(-P)s_j - C(P)s_{j+1}), \quad (8c)$$

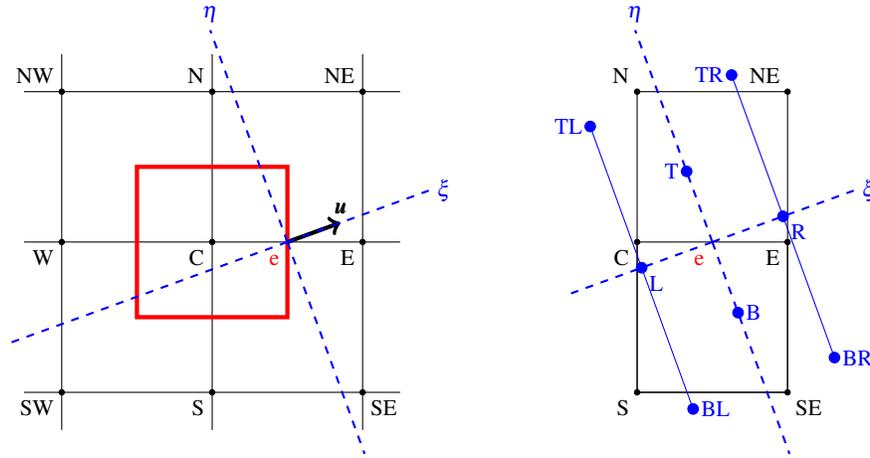
where  $P = u\Delta x/\varepsilon$  is the constant (grid) Péclet number. In the expressions in (8) we have introduced the functions  $B$  and  $C$  defined by  $B(z) = z/(e^z - 1)$  and  $C(z) = (e^{z/2} - 1 - z/2)/(z(e^z - 1))$ . In the special case that  $P = 0$ , i.e., there is no flow, the fluxes in (8) reduce to

$$F_{j+1/2}^h = \frac{\varepsilon}{\Delta x} (\varphi_j - \varphi_{j+1}), \quad F_{j+1/2}^i = \frac{1}{8} \Delta x (s_j - s_{j+1}). \quad (9)$$

The homogeneous flux in (9) is the central difference approximation of the diffusive flux  $f^d = -\varepsilon d\varphi/dx$ , and  $F_{j+1/2}^i = \mathcal{O}(\Delta x^2)$  for  $\Delta x \rightarrow 0$ , provided  $s$  is sufficiently smooth. In this case we may omit the inhomogeneous component.

### 3 Two-dimensional complete flux scheme

In this section we present an extension of the one-dimensional numerical flux to two-dimensional conservation laws. The basic idea is to decompose the normal component of the numerical flux vector at a cell interface into a component aligned with the (local) velocity field and a component perpendicular to it. We assume that  $\varepsilon$  is constant.



**Fig. 1** Control volume and local coordinate system for the computation of  $F_{x,e}$  (left) and stencil (right). Function values at locations L, R, B, T, TL, BL, TR, BR are found by interpolation/extrapolation, see (18).

Consider as an example the computation of the numerical flux component  $F_{x,e} = F_{x,i+1/2,j}$  at the eastern cell interface of the control volume, see Fig. 1 where we adopt the compass notation to denote the location of interface/grid points. Suppose, the basis vector  $\mathbf{e}_x$  and the local flow velocity  $\mathbf{u} = \mathbf{u}(\mathbf{x}_e)$  enclose an angle  $\alpha = \alpha(\mathbf{x}_e)$  ( $-\pi < \alpha \leq \pi$ ), oriented counter-clockwise, given by  $\tan(\alpha) = v(\mathbf{x}_e)/u(\mathbf{x}_e)$ . Based on the flow velocity at  $\mathbf{x}_e$  we introduce a local orthogonal coordinate system, denoted by  $(\xi, \eta)$ , and corresponding basis  $\{\mathbf{e}_\xi, \mathbf{e}_\eta\}$  according to

$$\mathbf{e}_\xi = \cos(\alpha)\mathbf{e}_x + \sin(\alpha)\mathbf{e}_y, \quad \mathbf{e}_\eta = -\sin(\alpha)\mathbf{e}_x + \cos(\alpha)\mathbf{e}_y. \quad (10)$$

The transformation between the position vectors  $\mathbf{x} = x\mathbf{e}_x + y\mathbf{e}_y$  in Cartesian coordinates and  $\boldsymbol{\xi} = \xi\mathbf{e}_\xi + \eta\mathbf{e}_\eta$  in local coordinates is given by

$$\mathbf{x} - \mathbf{x}_e = \mathbf{R}(\alpha)\boldsymbol{\xi}, \quad \mathbf{R}(\alpha) = \begin{pmatrix} \cos \alpha & -\sin \alpha \\ \sin \alpha & \cos \alpha \end{pmatrix}. \quad (11)$$

Note that in the  $(\xi, \eta)$ -coordinate system the interface velocity  $\mathbf{u}(\mathbf{x}_e) = U\mathbf{e}_\xi$  with  $U = |\mathbf{u}(\mathbf{x}_e)| \geq 0$ , elsewhere  $\mathbf{u} = u_\xi\mathbf{e}_\xi + u_\eta\mathbf{e}_\eta$ .

We introduce  $\varphi^*(\xi, \eta) = \varphi(x, y)$ . Reformulated in the local, orthogonal  $(\xi, \eta)$ -coordinate system, the conservation law (1) and the expression (2) for the flux read

$$\nabla \cdot \mathbf{f} = \frac{\partial f_\xi}{\partial \xi} + \frac{\partial f_\eta}{\partial \eta} = s, \quad (12a)$$

$$\mathbf{f} = f_\xi\mathbf{e}_\xi + f_\eta\mathbf{e}_\eta = \left(u_\xi\varphi^* - \varepsilon\frac{\partial\varphi^*}{\partial\xi}\right)\mathbf{e}_\xi + \left(u_\eta\varphi^* - \varepsilon\frac{\partial\varphi^*}{\partial\eta}\right)\mathbf{e}_\eta. \quad (12b)$$

The expression for the flux at the interface reduces to

$$\mathbf{f}(\mathbf{x}_e) = \left(U\varphi^* - \varepsilon\frac{\partial\varphi^*}{\partial\xi}\right)\mathbf{e}_\xi - \varepsilon\frac{\partial\varphi^*}{\partial\eta}\mathbf{e}_\eta. \quad (13)$$

In the following we omit the asterisk (\*). Note that  $f_x = \cos(\alpha)f_\xi - \sin(\alpha)f_\eta$ , thus to compute  $F_{x,e}$  we need numerical approximations  $F_{\xi,e}$  and  $F_{\eta,e}$  of the flux components  $f_\xi(\mathbf{x}_e)$  and  $f_\eta(\mathbf{x}_e)$ , respectively.

First, consider the computation of the component  $F_{\xi,e}$ . Similar to the derivation of the one-dimensional flux, we determine  $F_{\xi,e}$  from the following local quasi-one-dimensional BVP:

$$\frac{\partial f_\xi}{\partial \xi} = \frac{\partial}{\partial \xi} \left( U\varphi - \varepsilon\frac{\partial\varphi}{\partial\xi} \right) = s_\xi, \quad -\frac{1}{2}h < \xi < \frac{1}{2}h, \eta = 0, \quad (14a)$$

$$\varphi(-\frac{1}{2}h, 0) = \varphi_L, \quad \varphi(\frac{1}{2}h, 0) = \varphi_R, \quad (14b)$$

where we choose  $h = \min(\Delta x, \Delta y)$ . Equation (14a) is a reformulation of the conservation law (12a), defined on the line segment connecting  $\mathbf{x}_L = \mathbf{x}_e - \frac{1}{2}h\mathbf{e}_\xi$  and  $\mathbf{x}_R = \mathbf{x}_e + \frac{1}{2}h\mathbf{e}_\xi$ , with the flow velocity  $\mathbf{u}$  replaced by  $U\mathbf{e}_\xi$  and where the right hand side function  $s_\xi$  is a modified source term containing an approximation of the cross

flux  $f_\eta$ . It is given by

$$s_\xi = s(\mathbf{x}(\xi, 0)) + \varepsilon \delta_{\eta\eta} \varphi(\mathbf{x}(\xi, 0)), \quad (15)$$

with  $\delta_{\eta\eta} \varphi$  the standard central difference approximation of  $\partial^2 \varphi / \partial \eta^2$ . Note that the boundary values  $\varphi_L = \varphi(\mathbf{x}_L)$  (left) and  $\varphi_R = \varphi(\mathbf{x}_R)$  (right) are not grid point values and need to be approximated by interpolation. We will specify this shortly. Analogous to (8) we find the following expressions for the flux:

$$F_{\xi,e} = F_{\xi,e}^h + F_{\xi,e}^i, \quad (16a)$$

$$F_{\xi,e}^h = \frac{\varepsilon}{h} (B(-P)\varphi_L - B(P)\varphi_R), \quad (16b)$$

$$\begin{aligned} F_{\xi,e}^i &= h(C(-P)s_{\xi,L} - C(P)s_{\xi,R}) \\ &= h(C(-P)(s_L + \varepsilon \delta_{\eta\eta} \varphi_L) - C(P)(s_R + \varepsilon \delta_{\eta\eta} \varphi_R)), \end{aligned} \quad (16c)$$

with  $P = Uh/\varepsilon > 0$  the (local) grid Péclet number. Analogous to the previous, the numerical flux  $F_{\xi,e}$  is the sum of the homogeneous flux  $F_{\xi,e}^h$ , corresponding to the advection-diffusion operator in  $\xi$ -direction, and the inhomogeneous flux  $F_{\xi,e}^i$ , depending on source and cross flux.

Next, for the (diffusive) component  $F_{\eta,e}$  we adopt the standard central difference scheme for the homogeneous part and discard the inhomogeneous part; cf. (9). Introducing the auxiliary points  $\mathbf{x}_B = \mathbf{x}_e - \frac{1}{2}h\mathbf{e}_\eta$  (bottom) and  $\mathbf{x}_T = \mathbf{x}_e + \frac{1}{2}h\mathbf{e}_\eta$  (top), it is given by

$$F_{\eta,e} = F_{\eta,e}^h = \frac{\varepsilon}{h} (\varphi_B - \varphi_T), \quad (17)$$

where  $\varphi_B = \varphi(\mathbf{x}_B)$  and  $\varphi_T = \varphi(\mathbf{x}_T)$  need to be determined by interpolation.

To determine the auxiliary function values in (16) and (17) we need interpolation; see Fig. 1. Since  $\mathbf{x}_L$ ,  $\mathbf{x}_R$ ,  $\mathbf{x}_B$  and  $\mathbf{x}_T$  are all located in the rectangle  $\mathcal{R}(\mathbf{x}_e) = [x_C, x_E] \times [y_S, y_N]$  with vertices NE, N, S and SE, centered around  $\mathbf{x}_e$ , we use linear interpolation in  $x$ -direction and quadratic interpolation in  $y$ -direction for  $(x, y) \in \mathcal{R}(\mathbf{x}_e)$ . Let  $p$  be the interpolation polynomial, then we have for example  $\varphi_L = p(\mathbf{x}_L)$ . Introducing the scaled coordinates  $\sigma_x$  ( $0 \leq \sigma_x \leq 1$ ) and  $\sigma_y$  ( $-1 \leq \sigma_y \leq 1$ ) according to  $\sigma_x(x) = (x - x_C)/\Delta x$ ,  $\sigma_y(y) = (y - y_C)/\Delta y$ , the interpolation polynomial  $p$  can be written as

$$p(x, y) = [1 - \sigma_x \quad \sigma_x] \begin{bmatrix} \varphi_S & \varphi_C & \varphi_N \\ \varphi_{SE} & \varphi_E & \varphi_{NE} \end{bmatrix} \begin{bmatrix} -\frac{1}{2}\sigma_y(1 - \sigma_y) \\ (1 - \sigma_y^2) \\ \frac{1}{2}\sigma_y(1 + \sigma_y) \end{bmatrix} = \sum_{Q \in \mathcal{N}(\mathbf{x}_e)} a_Q(\mathbf{x}) \varphi_Q, \quad (18)$$

where  $\mathcal{N}(\mathbf{x}_e) = \{N, NE, C, E, S, SE\}$ . Applying this interpolation formula to all  $\varphi$ -values in (16) and (17) and rearranging terms, we find the following expressions for the numerical flux:

$$F_{\xi,e}^h = \frac{\varepsilon}{h} \sum_{Q \in \mathcal{N}(\mathbf{x}_e)} (B(-P)a_Q(\mathbf{x}_L) - B(P)a_Q(\mathbf{x}_R)) \varphi_Q, \quad (19a)$$

$$F_{\xi,e}^i = h\varepsilon \sum_{Q \in \mathcal{N}(\mathbf{x}_e)} (C(-P)\delta_{\eta\eta}a_Q(\mathbf{x}_L) - C(P)\delta_{\eta\eta}a_Q(\mathbf{x}_R)) \varphi_Q \\ + h(C(-P)s_L - C(P)s_R), \quad (19b)$$

$$F_{\eta,e} = \frac{\varepsilon}{h} \sum_{Q \in \mathcal{N}(\mathbf{x}_e)} (a_Q(\mathbf{x}_B) - a_Q(\mathbf{x}_T)) \varphi_Q. \quad (19c)$$

Note that the central difference approximations  $\delta_{\eta\eta}a_Q(\mathbf{x}_L)$  and  $\delta_{\eta\eta}a_Q(\mathbf{x}_R)$  in the expression for the inhomogeneous flux  $F_{\xi,e}^i$  contain function values in the points  $\mathbf{x}_L \pm h\mathbf{e}_\eta$  and  $\mathbf{x}_R \pm h\mathbf{e}_\eta$ , which are outside  $\mathcal{R}(\mathbf{x}_e)$ . For these values we still apply (18) (extrapolation). Finally, the numerical flux is then given by  $F_{x,e} = \cos(\alpha)F_{\xi,e} - \sin(\alpha)F_{\eta,e}$ , and depends on the six grid point values  $\varphi_Q$  with  $Q \in \mathcal{N}(\mathbf{x}_e)$ . A similar procedure can be applied to all other numerical fluxes, and substituting these in (4) gives rise to the 9-point stencil shown in Fig. 1.

## 4 Numerical results

We have applied the complete flux scheme to equation (1) for two different flow velocities, viz. a constant velocity field  $\mathbf{u}(x,y) = u\mathbf{e}_x + v\mathbf{e}_y$ , not aligned with the grid and  $\mathbf{u}(x,y) = 2y(1-x^2)\mathbf{e}_x - 2x(1-y^2)\mathbf{e}_y$ , corresponding to rotating flow.

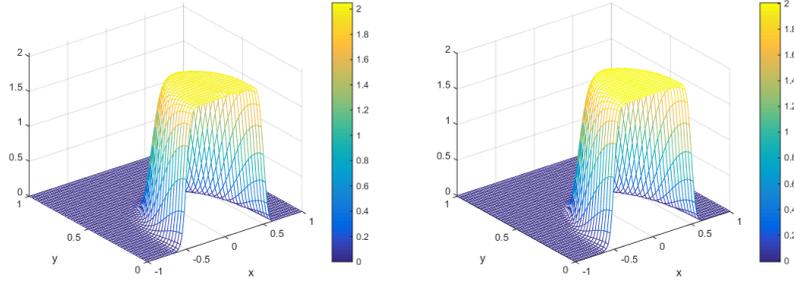
For the first case, we set  $s(x,y) = (x-1)(x+1)y(y-1)$ , take several values of the angle  $\alpha$  and vary  $\varepsilon$  from 1 to  $10^{-8}$ . To determine the order of convergence, we choose  $\Delta x = \Delta y = h$  and apply Richardson extrapolation to the numerical solution at location  $(\frac{1}{2}, \frac{1}{2})$ . We always obtain order 2 in the limit  $h \rightarrow 0$ , uniformly in  $\varepsilon$ , see the results in Table 1.

The second flow velocity comes from a benchmark problem by Smith and Hutton [3]; see also Example 3 in [4]. In this problem an inlet profile with steep layer defined for  $-1 \leq x \leq 0$  and  $y = 0$  is convected around a  $180^\circ$  degree bend to the outlet ( $0 < x \leq 1$  and  $y = 0$ ). There is no source. We have computed numerical solutions for  $\varepsilon = 10^{-8}$  on a coarse  $80 \times 40$  grid using the CF-scheme as well as

$h^{-1}$	$\varepsilon = 1$	$\varepsilon = 10^{-2}$	$\varepsilon = 10^{-8}$	$h^{-1}$	$\varepsilon = 1$	$\varepsilon = 10^{-2}$	$\varepsilon = 10^{-8}$
40	3.7156	1.0432	0.0705	40	4.0706	1.3677	3.5803
80	3.8493	2.9941	2.2333	80	4.0351	2.2128	3.7470
160	3.9230	3.7650	3.0759	160	4.0175	2.9808	3.9053
320	3.9611	3.9790	3.5871	320	4.0087	3.7679	3.9603
640	3.9805	4.0127	3.8014	640	4.0044	3.7679	3.9821

**Table 1** Values for  $r_h := (\varphi_{h/2} - \varphi_h) / (\varphi_{h/4} - \varphi_{h/2}) \approx 2^p$  with  $\varphi_h$  the numerical approximation of  $\varphi(\frac{1}{2}, \frac{1}{2})$  computed with grid size  $h$  and  $p$  the convergence order. Left:  $u = -1, v = \sqrt{2}/2$ . Right:  $u = 1, v = 1$ .

the homogeneous flux (HF) scheme, ignoring the inhomogeneous flux (16c); see Fig. 2. Both schemes produce a sharp resolution of the interior layer. Comparing these solutions to the standard HF solution presented in [4], which flattens out the profile, we conclude that the schemes in local  $(\xi, \eta)$ -coordinates do not suffer from numerical diffusion.



**Fig. 2** Numerical solution of the rotating flow problem, computed with the CF (left) and HF (right) scheme. The grid size  $\Delta x = \Delta y = 2.5 \times 10^{-2}$ .

## 5 Concluding remarks

We have presented a version of the two-dimensional complete flux scheme in terms of local, orthogonal flow adapted coordinates. The scheme involves a flux component  $F_\xi$  parallel to the local velocity field and a component  $F_\eta$  perpendicular to it. For  $F_\xi$  we employ the one-dimensional complete flux approximation, including the cross flux, whereas for  $F_\eta$  the homogeneous flux scheme suffices. The resulting finite volume scheme exhibits uniform second order convergence and does not suffer from numerical diffusion. This approach is readily generalized to three-dimensional problems, which will be presented in future work.

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