Harmonic Complete Flux Schemes for Conservation Laws with Discontinuous Coefficients

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Abstract In this paper we discuss several complete flux schemes for advection-diffusion-reaction problems. We consider both scalar equations as well as systems of equations. For the flux approximations in the latter case, we take into account the coupling between the constituent equations. We study conservation laws with discontinuous diffusion matrix/coefficient and show that the (matrix) harmonic average should be employed in the expressions for the numerical fluxes. The vectorial harmonic complete flux schemes are validated for a test problem.

1 Introduction

Conservation laws are ubiquitous in continuum physics. They occur in disciplines like combustion theory, plasma physics, transport in porous media etc. These conservation laws are often of advection-diffusion-reaction type, describing the interplay between different processes such as advection or drift, (multi-species) diffusion and chemical reactions or impact ionization.

Advection-diffusion-reaction problems are usually quite complex and require sophisticated numerical solution methods. In this contribution we discuss numerical flux approximations for two special cases: first, a scalar conservation law with a rapidly varying or even discontinuous diffusion coefficient, and second, a system of conservation laws coupled through a diffusion matrix. We also allow the diffusion matrix to be discontinuous. The second problem is typical for multi-species diffusion in mixtures or plasmas; see for example [3] for a detailed account.

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Due to the nonlinear dependency of the diffusion process on pressure, temperature and plasma composition, diffusion matrices can vary rapidly in space.

Therefore, we consider the one-dimensional scalar model problem $\mathrm{d}f/\mathrm{d}x = s$, where f is the (advection-diffusion) flux and s the source term. The flux f is given by

$$f = u\varphi - \varepsilon\frac{\mathrm{d}\varphi}{\mathrm{d}x}, \tag{1}$$

with u the advection velocity and $\varepsilon > 0$ the diffusion coefficient. The system counterpart reads $\mathrm{d}\boldsymbol{f}/\mathrm{d}x = \boldsymbol{s}$ with $\boldsymbol{f}$ the flux vector given by

$$\boldsymbol{f} = \boldsymbol{U}\boldsymbol{\varphi} - \mathscr{E}\frac{\mathrm{d}\boldsymbol{\varphi}}{\mathrm{d}x}, \tag{2}$$

and $\boldsymbol{s}$ the source term. In relation (2) $\boldsymbol{U}$ is the advection matrix, which is usually diagonal, and $\mathscr{E}$ is the diffusion matrix, which we assume symmetric positive definite. We consider equations with ε and $\mathscr{E}$ discontinuous.

The finite volume method is our discretization method of choice. Thus we cover the domain with a finite set of control volumes (cells) I_j of size Δx and choose the grid points x_j, where the unknown has to be approximated, in the cell centres. Consequently, we have $I_j = [x_{j-1/2}, x_{j+1/2}]$ with $x_{j+1/2} = \frac{1}{2}\big(x_j + x_{j+1}\big)$. Integrating, for example, $\mathrm{d}\boldsymbol{f}/\mathrm{d}x = \boldsymbol{s}$ over I_j and applying the midpoint rule for the integral of $\boldsymbol{s}$, we obtain the discrete conservation law

$$\boldsymbol{F}_{j+1/2} - \boldsymbol{F}_{j-1/2} = \Delta x\, \boldsymbol{s}_j, \tag{3}$$

with $\boldsymbol{F}_{j+1/2}$ the numerical flux approximating $\boldsymbol{f}$ at the cell interface $x_{j+1/2}$ and $\boldsymbol{s}_j = \boldsymbol{s}(x_j)$. For the numerical flux we adopt the complete flux schemes developed in [4, 5]. The complete flux schemes for $\boldsymbol{F}_{j+1/2}$ typically read

$$\boldsymbol{F}_{j+1/2} = \boldsymbol{\alpha}_{j+1/2}\boldsymbol{\varphi}_j - \boldsymbol{\beta}_{j+1/2}\boldsymbol{\varphi}_{j+1} + \Delta x(\boldsymbol{\gamma}_{j+1/2}\boldsymbol{s}_j + \boldsymbol{\delta}_{j+1/2}\boldsymbol{s}_{j+1}), \tag{4}$$

where $\boldsymbol{\varphi}_j$ denotes the numerical approximation of $\boldsymbol{\varphi}(x_j)$ and where the coefficient matrices $\boldsymbol{\alpha}_{j+1/2}$ etc. are piecewise constant and depend on $\boldsymbol{U}$ and $\mathscr{E}$. The goal of this paper is to extend the standard complete flux schemes to equations with discontinuous diffusion matrix/coefficient. We will deduce that the (matrix) harmonic average of the diffusion matrix/coefficient is required in the expressions for the numerical fluxes, which we collectively refer to as harmonic complete flux schemes.

We have organised our paper as follows. In Sect. 2 we modify the standard scalar complete flux scheme for piecewise constant diffusion coefficient ε. Next, in Sect. 3, we extend the scalar scheme to systems of conservation laws, taking into account the coupling between the constituent equations. In Sect. 4 we demonstrate the performance of the vectorial harmonic complete flux schemes, and finally we present conclusions in section “Concluding Remarks”.

2 Numerical Approximation of the Scalar Flux

In this section we outline the complete flux scheme for the scalar equation, which is based on the integral representation of the flux. The derivation is a modification of the theory in [4].

The integral representation of the flux $f(x_{j+1/2})$ at the cell edge $x_{j+1/2}$ is based on the following model boundary value problem (BVP) for φ:

$$\frac{\mathrm{d}}{\mathrm{d}x}\Big(u\varphi - \varepsilon\frac{\mathrm{d}\varphi}{\mathrm{d}x}\Big) = s, \quad x_j < x < x_{j+1}, \tag{5a}$$

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

We like to emphasize that $f(x_{j+1/2})$ corresponds to the solution of the inhomogeneous BVP (5), implying that $f(x_{j+1/2})$ not only depends on the advection-diffusion operator, but also on the source term s. It is convenient to introduce the variables $P(x)$, $p(x)$ and $S(x)$ for $x \in (x_j, x_{j+1})$ by

$$P(x) := \frac{u(x)\Delta x}{\varepsilon(x)}, \quad p(x) := \int_{x_{j+1/2}}^{x} \frac{u(\xi)}{\varepsilon(\xi)}\,\mathrm{d}\xi, \quad S(x) := \int_{x_{j+1/2}}^{x} s(\xi)\,\mathrm{d}\xi. \tag{6}$$

Here, $P(x)$ and $p(x)$ are the Peclet function and integral, respectively, generalizing the well-known (numerical) Peclet number. Integrating the differential equation $\mathrm{d}f/\mathrm{d}x = s$ from $x_{j+1/2}$ to $x \in [x_j, x_{j+1}]$ we get the integral balance $f(x) - f(x_{j+1/2}) = S(x)$. Using the definition of p in (6), it is clear that the flux can be rewritten as $f(x) = -\varepsilon(x)\mathrm{e}^{p(x)}\,\mathrm{d}\big(\varphi\,\mathrm{e}^{-p(x)}\big)/\mathrm{d}x$. Substituting this representation into the integral balance and integrating from x_j to x_{j+1} we find the following expressions for the flux:

$$f(x_{j+1/2}) = f^{\mathrm{h}}(x_{j+1/2}) + f^{\mathrm{i}}(x_{j+1/2}), \tag{7a}$$

$$f^{\mathrm{h}}(x_{j+1/2}) = \big(\mathrm{e}^{-p(x_j)}\varphi_j - \mathrm{e}^{-p(x_{j+1})}\varphi_{j+1}\big) \Big/ \int_{x_j}^{x_{j+1}} \varepsilon^{-1}(x)\mathrm{e}^{-p(x)}\,\mathrm{d}x, \tag{7b}$$

$$f^{\mathrm{i}}(x_{j+1/2}) = -\int_{x_j}^{x_{j+1}} \varepsilon^{-1}(x)\mathrm{e}^{-p(x)}S(x)\,\mathrm{d}x \Big/ \int_{x_j}^{x_{j+1}} \varepsilon^{-1}(x)\mathrm{e}^{-p(x)}\,\mathrm{d}x, \tag{7c}$$

where $f^{\mathrm{h}}(x_{j+1/2})$ and $f^{\mathrm{i}}(x_{j+1/2})$ are the homogeneous and inhomogeneous part, corresponding to the homogeneous and particular solution of (5), respectively.

Next, we assume that u is constant and ε is piecewise constant on $(x_j, x_{j+1}]$, i.e., $u(x) = \bar{u}_{j+1/2} := \frac{1}{2}\big(u_j + u_{j+1}\big)$ and

$$\varepsilon(x) = \begin{cases} \varepsilon_j & \text{if} \quad x_j < x \le x_{j+1/2}, \\ \varepsilon_{j+1} & \text{if} \quad x_{j+1/2} < x \le x_{j+1}. \end{cases} \tag{8}$$

Consequently, the function $p(x)$ is piecewise linear. Likewise, in agreement with the finite volume discretization, we take s piecewise constant. Substituting these approximations in the integral representation (7), and evaluating all integrals involved, we obtain the numerical flux:

$$F_{j+1/2} = F^{\mathrm{h}}_{j+1/2} + F^{\mathrm{i}}_{j+1/2}, \tag{9a}$$

$$F^{\mathrm{h}}_{j+1/2} = \frac{\tilde{\varepsilon}_{j+1/2}}{\Delta x}\big(B(-\bar{P}_{j+1/2})\varphi_j - B(\bar{P}_{j+1/2})\varphi_{j+1}\big), \tag{9b}$$

$$F^{\mathrm{i}}_{j+1/2} = \Delta x\big(\gamma_{j+1/2}s_j + \delta_{j+1/2}s_{j+1}\big), \tag{9c}$$

$$\gamma_{j+1/2} = \tfrac{1}{2}\frac{\psi\big(-\tfrac{1}{2}P_j\big)}{\mathrm{e}^{-\bar{P}_{j+1/2}} - 1}, \quad \delta_{j+1/2} = -\tfrac{1}{2}\frac{\psi\big(\tfrac{1}{2}P_{j+1}\big)}{\mathrm{e}^{\bar{P}_{j+1/2}} - 1}, \tag{9d}$$

where $\tilde{\varepsilon}_{j+1/2}$ is the harmonic average of ε and $\bar{P}_{j+1/2}$ the arithmetic average of P, defined by

$$\frac{1}{\tilde{\varepsilon}_{j+1/2}} := \frac{1}{2}\Big(\frac{1}{\varepsilon_j} + \frac{1}{\varepsilon_{j+1}}\Big), \quad \bar{P}_{j+1/2} := \frac{\bar{u}_{j+1/2}\Delta x}{\tilde{\varepsilon}_{j+1/2}}. \tag{10}$$

Furthermore, the functions $B(z)$ and $\psi(z)$ in (9) are defined by $B(z) = z/\big(\mathrm{e}^z - 1\big)$ and $\psi(z) = \big(\mathrm{e}^z - 1 - z\big)/z$. The flux approximation in (9) is referred to as the piecewise constant complete flux scheme (PCCFS).

Alternatively, we propose to replace the (local) Peclet numbers P_j and P_{j+1} in (9d) by the average Peclet number $\bar{P}_{j+1/2}$. This way we obtain

$$\gamma_{j+1/2} = W_1\big(\bar{P}_{j+1/2}\big), \quad \delta_{j+1/2} = -W_1\big(-\bar{P}_{j+1/2}\big), \tag{11}$$

with $W_1(z) = \big(\mathrm{e}^{-z/2} - 1 + z/2\big)/\big(z\big(1 - \mathrm{e}^{-z}\big)\big)$. The corresponding flux approximation is referred to as the harmonic complete flux scheme (HCF).

3 Extension to Systems of Conservation Laws

In this section we extend the derivation of the complete flux schemes to systems of conservation laws. The derivation is a modification of the theory in [5] and is detailed in [2].

Analogous to the scalar case, we derive the expression for the numerical flux $\boldsymbol{F}_{j+1/2}$ from the following system BVP:

$$\frac{\mathrm{d}}{\mathrm{d}x}\Big(\boldsymbol{U}\boldsymbol{\varphi} - \mathscr{E}\frac{\mathrm{d}\boldsymbol{\varphi}}{\mathrm{d}x}\Big) = \boldsymbol{s}, \quad x_j < x < x_{j+1}, \tag{12a}$$

$$\boldsymbol{\varphi}(x_j) = \boldsymbol{\varphi}_j, \quad \boldsymbol{\varphi}(x_{j+1}) = \boldsymbol{\varphi}_{j+1}, \tag{12b}$$

assuming that $\boldsymbol{U}(x) = \bar{\boldsymbol{U}}_{j+1/2} := \frac{1}{2}\big(\boldsymbol{U}_j + \boldsymbol{U}_{j+1}\big)$ is constant and $\mathscr{E}(x)$ is piecewise constant on $(x_j, x_{j+1}]$, i.e.,

$$\mathscr{E}(x) = \begin{cases} \mathscr{E}_j & \text{if} \quad x_j < x \leq x_{j+1/2}, \\ \mathscr{E}_{j+1} & \text{if} \quad x_{j+1/2} < x \leq x_{j+1}. \end{cases} \tag{13}$$

Recall that $\mathscr{E}$ is symmetric positive definite, and thus regular. We assume the source term $\boldsymbol{s}(x)$ to be piecewise constant. Let m denote the size of the system, thus $\boldsymbol{\varphi}$ and $\boldsymbol{s}$ are m-vectors and $\boldsymbol{U}$ and $\mathscr{E}$ are $m \times m$ matrices.

For the derivation which follows it is convenient to introduce the variables

$$\boldsymbol{A}(x) := \mathscr{E}^{-1}(x)\boldsymbol{U}, \quad \boldsymbol{P}(x) := \Delta x \boldsymbol{A}(x), \quad \boldsymbol{S}(x) := \int_{x_{j+1/2}}^{x} \boldsymbol{s}(\xi)\,\mathrm{d}\xi. \tag{14}$$

The matrix $\boldsymbol{P}$ is referred to as the Peclet matrix $\boldsymbol{P}$. Note that the matrices $\boldsymbol{A}$ and $\boldsymbol{P}$ are piecewise constant on $(x_j, x_{j+1}]$. Moreover, we assume that $\boldsymbol{A}$ has m real eigenvalues λ_i and m corresponding, linearly independent eigenvectors $\boldsymbol{v}_i$ $(i = 1, 2, \ldots, m)$. Since $\boldsymbol{A}$ has a complete set of eigenvectors, its spectral decomposition is given by

$$\boldsymbol{A}\boldsymbol{V} = \boldsymbol{V}\boldsymbol{\Lambda}, \quad \boldsymbol{\Lambda} := \mathrm{diag}\big(\lambda_1, \lambda_2, \ldots, \lambda_m\big), \quad \boldsymbol{V} := \big(\boldsymbol{v}_1, \boldsymbol{v}_2, \ldots, \boldsymbol{v}_m\big), \tag{15}$$

and based on this decomposition we can compute any matrix function of $\boldsymbol{P}$ as follows

$$g(\boldsymbol{P}) := \boldsymbol{V} g(\Delta x \boldsymbol{\Lambda})\boldsymbol{V}^{-1}, \quad g(\Delta x \boldsymbol{\Lambda}) := \mathrm{diag}(g(\Delta x \lambda_1), g(\Delta x \lambda_2), \ldots, g(\Delta x \lambda_m)), \tag{16}$$

provided g is defined on the spectrum of $\boldsymbol{A}$ [1].

Integrating the conservation law $\mathrm{d}\boldsymbol{f}/\mathrm{d}x = \boldsymbol{s}$ from the interface at $x_{j+1/2}$ to some arbitrary $x \in [x_j, x_{j+1}]$, we obtain

$$\boldsymbol{f}(x) - \boldsymbol{f}\big(x_{j+1/2}\big) = \boldsymbol{S}(x). \tag{17}$$

Next, we substitute the integrating factor formulation of the flux, which for $x \neq x_{j+1/2}$ is given by

$$\boldsymbol{f}(x) = -\mathscr{E} \mathrm{e}^{(x - x_{j+1/2})\boldsymbol{A}} \frac{\mathrm{d}}{\mathrm{d}x}\big(\mathrm{e}^{-(x - x_{j+1/2})\boldsymbol{A}} \boldsymbol{\varphi}\big) \tag{18}$$

in (17), isolate the derivative and subsequently integrate over the interval $[x_j, x_{j+1}]$ to obtain the integral formulation of the flux

$$\int_{x_j}^{x_{j+1}} \mathrm{e}^{-(x-x_{j+1/2})\boldsymbol{A}} \mathscr{E}^{-1}(x)\,\mathrm{d}x\, \boldsymbol{f}(x_{j+1/2}) = \\ \mathrm{e}^{\boldsymbol{P}_j/2}\boldsymbol{\varphi}_j - \mathrm{e}^{-\boldsymbol{P}_{j+1/2}}\boldsymbol{\varphi}_{j+1} - \int_{x_j}^{x_{j+1}} \mathrm{e}^{-(x-x_{j+1/2})\boldsymbol{A}} \mathscr{E}^{-1}(x)\boldsymbol{S}(x)\,\mathrm{d}x, \tag{19}$$

where $\boldsymbol{P}_j = \boldsymbol{P}(x_j)$ etc. In the right hand side, the first two terms correspond to the advection-diffusion operator whereas the integral corresponds to the source term. In order to determine the numerical flux we have to evaluate both integrals in (19).

Consider first the integral in the left hand side of (19) and take $\boldsymbol{S}(x) = \boldsymbol{0}$. Since $\mathscr{E}$ and $\boldsymbol{A}$ are piecewise constant, we split the integral in two parts and find the following relation for the homogeneous numerical flux $\boldsymbol{F}^{\mathrm{h}}_{j+1/2}$:

$$\tfrac{1}{2}\Delta x\Big(\big(\mathscr{E}_j B\big(\tfrac{1}{2}\boldsymbol{P}_j\big)\big)^{-1} + \big(\mathscr{E}_{j+1} B\big(-\tfrac{1}{2}\boldsymbol{P}_{j+1}\big)\big)^{-1}\Big)\boldsymbol{F}^{\mathrm{h}}_{j+1/2} = \\ \mathrm{e}^{\boldsymbol{P}_j/2}\boldsymbol{\varphi}_j - \mathrm{e}^{-\boldsymbol{P}_{j+1/2}}\boldsymbol{\varphi}_{j+1}. \tag{20}$$

Note that this expression is properly defined since the matrices $B\big(\tfrac{1}{2}\boldsymbol{P}_j\big)$ and$B\big(-\tfrac{1}{2}\boldsymbol{P}_{j+1}\big)$ are always regular. Next, consider the integral in the right hand side of (19). Since $\boldsymbol{S}(x)$ is piecewise linear, we can also evaluate this integral. Omitting the first two terms in the right hand side of (19) we obtain the following expression for the inhomogeneous flux $\boldsymbol{F}^{\mathrm{i}}_{j+1/2}$:

$$\Big(\big(\mathscr{E}_j B\big(\tfrac{1}{2}\boldsymbol{P}_j\big)\big)^{-1} + \big(\mathscr{E}_{j+1} B\big(-\tfrac{1}{2}\boldsymbol{P}_{j+1}\big)\big)^{-1}\Big)\boldsymbol{F}^{\mathrm{i}}_{j+1/2} = \\ -\tfrac{1}{2}\Delta x\Big(W_2\big(\tfrac{1}{2}\boldsymbol{P}_j\big)\mathscr{E}_j^{-1}\boldsymbol{s}_j - W_2\big(-\tfrac{1}{2}\boldsymbol{P}_{j+1}\big)\mathscr{E}_{j+1}^{-1}\boldsymbol{s}_{j+1}\Big), \tag{21}$$

where $W_2(z) = \big(\mathrm{e}^z(1-z)-1\big)/z^2$. The complete flux approximation is obviously given by $\boldsymbol{F}_{j+1/2} = \boldsymbol{F}^{\mathrm{h}}_{j+1/2} + \boldsymbol{F}^{\mathrm{i}}_{j+1/2}$, referred to as the piecewise constant complete flux scheme (PCCFS).

PCCFS is a rather complicated and expensive scheme, and therefore we propose the following approximation. Assume first that $\boldsymbol{U}$ is regular, then we can rewrite the expression (20) for the homogeneous flux as

$$\Big(\mathrm{e}^{\boldsymbol{P}_j/2} - \mathrm{e}^{-\boldsymbol{P}_{j+1/2}}\Big)\boldsymbol{U}^{-1}\boldsymbol{F}^{\mathrm{h}}_{j+1/2} = \mathrm{e}^{\boldsymbol{P}_j/2}\boldsymbol{\varphi}_j - \mathrm{e}^{-\boldsymbol{P}_{j+1/2}}\boldsymbol{\varphi}_{j+1}. \tag{22}$$

In general the Peclet matrices in (22) do not commute, so that we have to invoke the Baker-Campbell-Hausdorff formula [1], e.g.,

$$\mathrm{e}^{-\boldsymbol{P}_j/2}\mathrm{e}^{-\boldsymbol{P}_{j+1/2}} = \mathrm{e}^{-\bar{\boldsymbol{P}}_{j+1/2}+\frac{1}{8}\Delta x^2[\boldsymbol{A}_j,\boldsymbol{A}_{j+1}]+\mathscr{O}(\Delta x^3)}, \tag{23}$$

where $[\boldsymbol{A}_j, \boldsymbol{A}_{j+1}] := \boldsymbol{A}_j\boldsymbol{A}_{j+1} - \boldsymbol{A}_{j+1}\boldsymbol{A}_j$ is the commutator of both matrices. Neglecting the $\mathcal{O}(\Delta x^2)$-term in the exponent we can derive the vectorial equivalent of (9b), i.e.,

$$\boldsymbol{F}^{\mathrm{h}}_{j+1/2} = \frac{1}{\Delta x}\tilde{\mathscr{E}}_{j+1/2}\Big(B\big(-\bar{\boldsymbol{P}}_{j+1/2}\big)\boldsymbol{\varphi}_j - B\big(\bar{\boldsymbol{P}}_{j+1/2}\big)\boldsymbol{\varphi}_{j+1}\Big), \tag{24}$$

with $\tilde{\mathscr{E}}_{j+1/2}$ and $\bar{P}_{j+1/2}$ the matrix harmonic average of $\mathscr{E}$ and the average Peclet matrix, respectively, defined by

$$\tilde{\mathscr{E}}^{-1}_{j+1/2} := \tfrac{1}{2}\big(\mathscr{E}^{-1}_j + \mathscr{E}^{-1}_{j+1}\big), \quad \bar{\boldsymbol{P}}_{j+1/2} := \Delta x\tilde{\mathscr{E}}^{-1}_{j+1/2}\bar{\boldsymbol{U}}_{j+1/2}, \tag{25}$$

where obviously $\mathscr{E}^{-1}_j = \mathscr{E}^{-1}(x_j)$ etc.

In case $\boldsymbol{U}$ is singular, and consequently also $\boldsymbol{A}$, we apply a regularization technique to derive (24). Therefore, we replace $\boldsymbol{A}$ by a perturbation $\boldsymbol{A}_\delta = \boldsymbol{A} + \delta\boldsymbol{I}$ for some δ such that $\boldsymbol{A}_\delta$ is regular. This is possible, provided $-\delta \notin \sigma(\boldsymbol{A})$. The matrices $\boldsymbol{P}_\delta$ and $\bar{\boldsymbol{P}}_{\delta,j+1/2}$ are the corresponding perturbations of $\boldsymbol{P}$ and $\bar{\boldsymbol{P}}_{j+1/2}$, respectively. Replacing $\boldsymbol{P}$ by $\boldsymbol{P}_\delta$ in (20) we obtain a similar expression as (24) with $\bar{\boldsymbol{P}}_{\delta,j+1/2}$ instead of $\bar{\boldsymbol{P}}_{j+1/2}$. Since $B(z)$ is continuous for $z = 0$ we can take the limit $\delta \to 0$ to arrive at the expression (24).

Next, for the inhomogeneous flux, we take for $\mathscr{E}$ its matrix harmonic average $\tilde{\mathscr{E}}_{j+1/2}$ and evaluate the integral in the right hand side of (19) to obtain

$$\boldsymbol{F}^{\mathrm{i}}_{j+1/2} = \Delta x\big(W_1\big(\hat{\boldsymbol{P}}_{j+1/2}\big)\boldsymbol{s}_j - W_1\big(-\hat{\boldsymbol{P}}_{j+1/2}\big)\boldsymbol{s}_{j+1}\big), \tag{26}$$

with $\hat{\boldsymbol{P}}_{j+1/2} := \Delta x\bar{\boldsymbol{U}}_{j+1/2}\tilde{\mathscr{E}}^{-1}_{j+1/2}$; for more details see [2]. The resulting complete flux approximation $\boldsymbol{F}_{j+1/2} = \boldsymbol{F}^{\mathrm{h}}_{j+1/2} + \boldsymbol{F}^{\mathrm{i}}_{j+1/2}$ with $\boldsymbol{F}^{\mathrm{h}}_{j+1/2}$ and $\boldsymbol{F}^{\mathrm{i}}_{j+1/2}$ defined in (24) and (26), respectively, is referred to as the harmonic complete flux scheme (HCFS), as opposed to the standard complete flux scheme, which employs the arithmetic average of the diffusion matrix.

4 Numerical Example

As an example, we apply the vectorial complete flux schemes to the following test problem:

$$\frac{\mathrm{d}}{\mathrm{d}x}\Big(\boldsymbol{U}\boldsymbol{\varphi} - \mathscr{E}\frac{\mathrm{d}\boldsymbol{\varphi}}{\mathrm{d}x}\Big) = \boldsymbol{s}, \quad 0 < x < 1, \tag{27a}$$

$$\frac{\mathrm{d}\varphi_1}{\mathrm{d}x}(0) = 0,\ \varphi_1(1) = \varphi_{1,\mathrm{R}},\ \varphi_2(0) = \varphi_{2,\mathrm{L}},\ \frac{\mathrm{d}\varphi_2}{\mathrm{d}x}(1) = 0, \tag{27b}$$

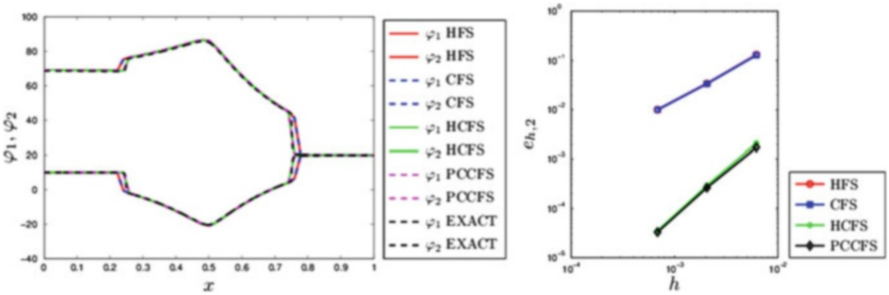

Fig. 1 Numerical solution of (27) (*left*) and discretization errors (*right*). Parameter values are: $u_1 = -1$, $u_2 = 1$, $\alpha = 0.05$ and $s_{\max} = 10^3$. Disretization schemes employed are: standard complete scheme (*CFS*), homogeneous flux scheme (*HFS*), PCCFS and HCFS

with $\boldsymbol{U} = \mathrm{diag}(u_1, u_2)$ and where the diffusion matrix $\mathscr{E}$ and the source term vector $\boldsymbol{s}$ are given by

$$\mathscr{E} = \tfrac{1}{2}\varepsilon \begin{pmatrix} 1+\alpha & 1-\alpha \\ 1-\alpha & 1+\alpha \end{pmatrix}, \quad \varepsilon(x) = \begin{cases} 10^{-2} & \text{if} \quad x \in [0, 0.25) \\ 1 & \text{if} \quad x \in [0.25, 0.75) \\ 10^{-2} & \text{if} \quad x \in [0.75, 1) \end{cases}, \tag{27c}$$

$$\boldsymbol{s}(x) = \frac{s_{\max}}{1 + s_{\max}(2x-1)^2} \begin{pmatrix} 1 \\ 0.2 \end{pmatrix}. \tag{27d}$$

The problem is diffusion dominant in the middle, in $(0.25, 0.75)$, and advection dominant in the remainder of the domain. The parameter α $(0 \leq \alpha \leq 1)$ determines the coupling between the constituent equations of (27a). The source term has a sharp peak at $x = 0.5$ causing steep interior layers near the discontinuities of ε. A typical solution of (27) is displayed in Fig. 1.

To assess the (order) of convergence of the numerical solutions we first compute a very fine grid solution $\boldsymbol{\varphi}^*$, which to good approximation equals the exact solution. An average discretization error for the second component φ_2, for example, is then given by $e_2(\Delta x) = \Delta x||\varphi_2^* - \varphi_2||_1$. In Fig. 1 this discretization error as function of the grid size Δx is plotted for various schemes. The standard complete flux and homogeneous flux schemes display only first order convergence, whereas HCFS and PCCFS are second order convergent and have a much smaller discretization error.

Concluding Remarks

In this contribution we have proposed several modifications of the standard complete flux schemes, both scalar and vectorial, for conservation laws with discontinuous diffusion matrix/coefficient. For the numerical flux

(continued)

approximations we employed the (matrix) harmonic average of the diffusion matrix/coefficient, which turned out to be more accurate than the standard schemes. However, more elaborate testing of the modified schemes for realistic applications, such as plasma simulations, is still required.

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