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The finite volume-complete flux scheme for one-dimensional advection-diffusion-reaction systems

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Abstract

We present the extension of the complete flux scheme to advection-diffusion-reaction systems. The flux approximation is derived from a local system boundary value problem for the entire system, including the source term vector. Therefore, the numerical flux vector consists of a homogeneous and an inhomogeneous component, corresponding to the homogeneous and the particular solution of the boundary value problem, respectively. The complete flux scheme is validated for a test problem and shows uniform second order convergence behaviour.

Keywords. Advection-diffusion-reaction systems, flux (vector), finite volume method, integral representation of the flux, Green’s matrix, numerical flux, matrix functions, Peclet matrix.

1 Introduction

Conservation laws are ubiquitous in continuum physics, they occur in disciplines like fluid mechanics, combustion theory, plasma physics, semiconductor physics etc. 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) reaction or recombination/generation. Examples are the conservation equations for reacting flow [9] or plasmas [11].

Diffusion in mixtures containing many species is often very complex. In particular, when there is no dominant species Fick’s law, stating that the diffusion velocity of a species is proportional to its concentration gradient, is often not adequate. Instead, the diffusion velocities of all species are coupled through the Stefan-Maxwell equations, relating the diffusion velocity of a species to the concentration gradients of all species; see e.g. [1] for a detailed description of multi-species diffusion. This coupling between diffusion velocities can be reformulated in terms of a diffusion matrix for the continuity equations; see [8]. Moreover, the advection/drift velocities of species in a mixture are often not the same, due to, e.g., different mobilities. Therefore, we consider as model problem a second order ODE system containing a diagonal advection matrix and a diffusion matrix as coefficients. The diffusion matrix is assumed to be symmetric, positive definite, and thus regular, the advection matrix can be singular.

The numerical solution of such system requires at least an adequate (space) discretisation. There are many (classes of) methods available, such as finite element, finite difference, finite volume or spectral methods. We restrict ourselves to finite volume methods; for a detailed account see e.g. [7, 16, 4]. Finite volume methods are based on the integral formulation, i.e., the equation (system) is integrated over a
disjunct set of control volumes covering the domain. The resulting discrete system involves fluxes at the interfaces of the control volumes, which need to be approximated. Our objective in this paper is to extend the complete flux scheme presented in [15] to advection-diffusion-reaction systems, thereby including the coupling between the constituent equations in the discretization.

The complete flux approximation, either scalar or vectorial, is derived from a local boundary value problem for the entire equation/system, including the source term (vector). As a consequence, the numerical flux is the superposition of a homogeneous and an inhomogeneous flux, corresponding to the homogeneous and the particular solution of the boundary value problem, respectively. The numerical flux vector closely resembles its scalar counterpart and is formulated in terms of matrix functions of the Peclet matrix $P$, generalizing the well-known (numerical/grid) Peclet number $P$. The inclusion of the inhomogeneous flux is important for dominant advection, since it ensures second order accuracy. For dominant diffusion the inhomogeneous flux is of little importance. The combined finite volume-complete flux scheme has a three-point coupling, resulting in a block-tridiagonal algebraic system which can be solved very efficiently, and virtually never generates spurious oscillations.

Coupled discretization schemes are very common for hyperbolic initial value problems, think of the Godunov scheme and all high resolution schemes based on it; see e.g. [12]. To our knowledge, there are very few coupled discretization schemes for advection-diffusion-reaction boundary value systems. Doolan et al. [3] discuss finite difference methods for second order ODE systems, where the coefficient of the second derivative is just a scalar. Another exception is the exponential fitting scheme in [13] for avalanche generation in semiconductors. In this publication, the coupling in the discretisation comes from the avalanche generation source term.

We have organised our paper as follows. The finite volume method is briefly summarized in Section 2. In Section 3 we outline the scalar version of the complete flux scheme, which is subsequently generalized to systems in Section 4. The combined finite volume-complete flux scheme is elaborated in Section 5. To test the scheme, we apply it in Section 6 to a test problem. Finally, we end with a summary and conclusions in Section 7.

## 2 Finite volume discretisation

In this section we outline the finite volume method (FVM) for a generic system of conservation laws of advection-diffusion-reaction type, restricting ourselves to stationary, one-dimensional problems. So, consider the following system defined on the interval $(0, 1)$

\[
(U \varphi - E \varphi)' = s, \tag{2.1}
\]

where $U = \text{diag}(u_1, u_2, \ldots, u_m)$ is the advection matrix, $E = (e_{ij})$ the diffusion matrix and $s$ a source term vector. The prime ($'$) denotes differentiation with respect to the spatial coordinate $x$. We assume that $E$ is symmetric, positive definite, and hence regular. The vector of unknowns $\varphi$ contains, e.g., the temperature and species mass fractions of a reacting flow or a plasma. Note that there is a coupling between the constituent equations of (2.1) through the diffusion matrix $E$, which is typical for multi-species diffusion as described, e.g., by the Stefan-Maxwell equations. The matrix $U$ represents the advection/drift velocities of the individual variables (species), which can differ because of different mobilities. The parameters $E$ and $s$ are usually (complicated) functions of the unknown $\varphi$, and $U$ has to be computed from (flow) equations accompanying (2.1), however, for the sake of discretisation, we consider these as given functions of $x$. 
3 NUMERICAL APPROXIMATION OF THE SCALAR FLUX

Associated with system (2.1) we introduce the flux vector \( f \), defined by
\[
f = U \varphi - E \varphi'.
\] (2.2)
System (2.1) then reduces to \( f' = s \). Integrating this system over an arbitrary interval \([\alpha, \beta] \subset [0, 1]\) we obtain the integral form of the conservation law, i.e.,
\[
f(\beta) - f(\alpha) = \int_{\alpha}^{\beta} s(x) \, dx.
\] (2.3)
In the FVM we cover \([0, 1]\) with a finite number of disjunct intervals (control volumes) \( I_j \) of size \( \Delta x \). Moreover, we have to define a spatial grid \( \{x_j\} \) where the variable \( \varphi \) has to be approximated. In this paper we choose the cell-centred approach [16], i.e., we choose the grid point \( x_j \) in the centre of the \( j \)th interval \( I_j \). Consequently we have \( I_j : = [x_{j-1/2}, x_{j+1/2}] \) with \( x_{j+1/2} := \frac{1}{2}(x_j + x_{j+1}) \). Imposing the integral form (2.3) on each of the intervals \( I_j \) and approximationg the integral in the right hand side by the midpoint rule, we obtain the discrete conservation law
\[
F_{j+1/2} - F_{j-1/2} = s_j \Delta x,
\] (2.4)
where \( F_{j+1/2} \) is the numerical flux (vector) approximating \( f \) at \( x = x_{j+1/2} \) and \( s_j := s(x_j) \). The FVM has to be completed with expressions for the numerical flux. We require that the numerical flux \( F_{j+1/2} \) linearily depends on \( \varphi \) and \( s \) in the neighbouring grid points \( x_j \) and \( x_{j+1} \), i.e., we are looking for an expression of the form
\[
F_{j+1/2} = \alpha \varphi_j - \beta \varphi_{j+1} + \Delta x (\gamma s_j + \delta s_{j+1}),
\] (2.5)
where the coefficient matrices \( \alpha \) etc. are piecewise constant and only depend on \( U \) and \( E \). Substitution of this expression in the discrete conservation law (2.4) leads to a block-tridiagonal linear system for the vector of unknowns.

The procedure to compute \( F_{j+1/2} \) is detailed in the next two sections. First, in Section 3 we outline the flux approximation for a scalar conservation law, and subsequently in Section 4, we extend the derivation to systems.

3 Numerical approximation of the scalar flux

In this section we present the complete flux scheme for the scalar flux, which is based on the integral representation of the flux. The derivation is a summary of the theory in [6].

The scalar conservation law can be written as \( f' = s \) with \( f = u \varphi - \varepsilon \varphi' \) (\( \varepsilon > 0 \)). The integral representation of the flux \( f_{j+1/2} = F(x_{j+1/2}) \) at the cell edge \( x_{j+1/2} \) located between the grid points \( x_j \) and \( x_{j+1} \) is based on the following model boundary value problem (BVP) for the variable \( \varphi \)
\[
\begin{align*}
(u \varphi - \varepsilon \varphi')' &= s, \quad x_j < x < x_{j+1}, \\
\varphi(x_j) &= \varphi_j, \quad \varphi(x_{j+1}) = \varphi_{j+1}.
\end{align*}
\] (3.1a,b)
In accordance with (2.5), we derive an expression for the flux \( f_{j+1/2} \) corresponding to the solution of the inhomogeneous BVP (3.1), implying that \( f_{j+1/2} \) not only depends on \( u \) and \( \varepsilon \), but also on the source term \( s \). It is convenient to introduce the variables \( a, P, A \) and \( S \) for \( x \in (x_j, x_{j+1}) \) by
\[
\begin{align*}
a &= \frac{u}{\varepsilon}, \quad P = a \Delta x, \quad A(x) = \int_{x_{j+1/2}}^{x} a(\xi) \, d\xi, \quad S(x) := \int_{x_{j+1/2}}^{x} s(\xi) \, d\xi.
\end{align*}
\] (3.2)
Here, $P$ and $A$ are the Peclet function and Peclet integral, respectively, generalizing the well-known (numerical) Peclet number. Integrating the differential equation (3.1a) from $x_{j+1/2}$ to $x$ we get the integral balance $f(x) - f_{j+1/2} = S(x)$. Using the definition of $A$ in (3.2), it is clear that the flux can be rewritten as $f = -\varepsilon e^A (e^{-A}\varphi)'$. Substituting this into the integral balance and integrating from $x_j$ to $x_{j+1}$ we obtain the following expression for the flux

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

(3.3a)

$$f_{j+1/2}^{(h)} = -\left(e^{-A_j\varphi_{j+1}} - e^{-A_j\varphi_j}\right) / \int_{x_j}^{x_{j+1}} \varepsilon^{-1} e^{-A} \, dx,$$

(3.3b)

$$f_{j+1/2}^{(i)} = -\int_{x_j}^{x_{j+1}} \varepsilon^{-1} e^{-A} S \, dx / \int_{x_j}^{x_{j+1}} \varepsilon^{-1} e^{-A} \, dx,$$

(3.3c)

where $f_{j+1/2}^{(h)}$ and $f_{j+1/2}^{(i)}$ are the homogeneous and inhomogeneous part, corresponding to the homogeneous and particular solution of (3.1), respectively.

In the following we assume that $u$ and $\varepsilon$ are constant, extension to variable coefficients is discussed in [6, 15]. In this case we can determine all integrals involved. Moreover, substituting the expression for $S(x)$ in (3.3c) and changing the order of integration, we can derive an alternative expression for the inhomogeneous flux. This way we obtain

$$f_{j+1/2}^{(h)} = \frac{\varepsilon}{\Delta x} \left( B(-P)\varphi_j - B(P)\varphi_{j+1} \right),$$

(3.4a)

$$f_{j+1/2}^{(i)} = \Delta x \int_{0}^{1} G(\sigma; P)s(x(\sigma)) \, d\sigma, \quad x(\sigma) = x_j + \sigma \Delta x.$$

(3.4b)

Here $B(z) = z/(e^z - 1)$ is the generating function of the Bernoulli numbers, in short Bernoulli function, see Figure 1, and $G(\sigma; P)$ the Green’s function for the flux, given by

$$G(\sigma; P) = \begin{cases} 
\frac{1 - e^{-P\sigma}}{1 - e^{-P}} & \text{for } 0 \leq \sigma \leq \frac{1}{2}, \\
\frac{1 - e^{P(1-\sigma)}}{1 - e^{P}} & \text{for } \frac{1}{2} < \sigma \leq 1;
\end{cases}$$

(3.5)

see Figure 2. Note that the homogeneous flux (3.4a) is the well-known exponential flux.
4 Numerical approximation of the flux vector

Next, we give the numerical flux \( F_{j+1/2} \). For the homogeneous component \( F_{j+1/2}^{(h)} \) we obviously take (3.4a), i.e., \( F_{j+1/2}^{(h)} = f_{j+1/2}^{(h)} \). The approximation of the inhomogeneous component \( f_{j+1/2}^{(i)} \) depends on \( P \). For dominant diffusion (\( |P| \ll 1 \)) the average value of \( G(\sigma; P) \) is small, which implies that the inhomogeneous flux is of little importance. On the contrary, for dominant advection (\( |P| \gg 1 \)), the average value of \( G(\sigma; P) \) on the half interval upwind of \( \sigma = \frac{1}{2} \), i.e., the interval \([0, \frac{1}{2}] \) for \( u > 0 \) and \([\frac{1}{2}, 1] \) for \( u < 0 \), is much larger than the average value on the downwind half. This means that for dominant advection the upwind value of \( s \) is the relevant one, and therefore we replace \( s(x(\sigma)) \) in (3.4b) by its upwind value \( s_{u,j+1/2} \), i.e., \( s_{u,j+1/2} = s_j \) if \( u \geq 0 \) and \( s_{u,j+1/2} = s_{j+1} \) if \( u < 0 \), and evaluate the resulting integral exactly. This way we obtain

\[
F_{j+1/2} = F_{j+1/2}^{(h)} + \left( \frac{1}{2} - W(P) \right) s_{u,j+1/2} \Delta x,
\]

where \( W(z) = (e^z - 1 - z)/(z(e^z - 1)) \); see Figure 1. From this expression it is once more clear that the inhomogeneous component is only of importance for dominant advection. We refer to (3.6) as the complete flux (CF) scheme, as opposed to the homogeneous flux (HF) scheme for which we ignore the inhomogeneous component.

4 Numerical approximation of the flux vector

We extend the derivation in the previous section to systems of conservation laws, including the coupling between the constituting equations in the discretisation. The representation of the flux vector turns out to be similar to its scalar counterpart.

Analogous to the scalar case, the integral representation of the flux vector \( f_{j+1/2} \) at the interface \( x = x_{j+1/2} \) is determined from the system BVP

\[
(U \varphi - \mathcal{E} \varphi')' = s, \quad x_j < x < x_{j+1},
\]
\[
\varphi(x_j) = \varphi_j, \quad \varphi(x_{j+1}) = \varphi_{j+1},
\]

where we assume that the matrices \( U \) and \( \mathcal{E} \) are constant. Recall that \( \mathcal{E} \) is regular, and even symmetric, positive definite, whereas \( U \) might be singular. In the derivation that follows, we need the following variables

\[
A := \mathcal{E}^{-1}U, \quad P := \Delta x A, \quad S(x) := \int_{x_{j+1/2}}^{x} s(\xi) d\xi;
\]
c.f. (3.2). We refer to \( P \) as the Peclet matrix, generalizing the Peclet number. We have to determine several matrix functions \( g(P) \) and the matrix sign function \( \text{sgn}(A) \), which depend on the eigenvalues and eigenvectors of \( A \). We restrict ourselves to the standard case, where \( A \) has \( m \) real eigenvalues \( \lambda_i \) and \( m \) corresponding, linearly independent, eigenvectors \( v_i \), satisfying the generalized eigenvalue problem

\[
(U - \lambda E)v = 0.
\]

Since \( A \) has a complete set of eigenvectors, its (spectral) decomposition is given by

\[
A = V \Lambda V^{-1}, \quad \Lambda := \text{diag}(\lambda_1, \lambda_2, \ldots, \lambda_m), \quad V := (v_1 \ v_2 \ \cdots \ v_m).
\]

Note that the matrices \( A \) and \( V \) are constant. Based on this decomposition, we can determine any matrix function \( g(P) \) that is defined on the spectrum of \( A \) and the matrix sign function \( \text{sgn}(A) \) as follows [5]

\[
g(P) = g(\Delta x A) = V g(\Delta x \Lambda)V^{-1},
\]

\[
g(\Delta x \Lambda) = \text{diag}(g(\Delta x \lambda_1), g(\Delta x \lambda_2), \ldots, g(\Delta x \lambda_m)),
\]

\[
\text{sgn}(A) = V \text{sgn}(\Lambda)V^{-1}, \quad \text{sgn}(\Lambda) = \text{diag}(\text{sgn}(\lambda_1), \text{sgn}(\lambda_2), \ldots, \text{sgn}(\lambda_m)).
\]

where we define \( \text{sgn}(0) = 1 \). Moreover, we need the following properties of matrix exponentials

\[
\left(e^{x A}ight)' = A e^{x A}, \quad A_1 e^{x A_1} = e^{x A_1} A_1, \quad \left(e^{x A}ight)^{-1} = e^{-x A},
\]

\[
A_1 A_2 = A_2 A_1 \Rightarrow e^{A_1+A_2} = e^{A_1} e^{A_2},
\]

for arbitrary matrices \( A_1 \) and \( A_2 \).

We can essentially repeat the derivation in Section 3. First, substituting the expression (2.2) in (4.1a) and integrating from \( x_{j+1/2} \) to \( x \) we get the integral balance

\[
f(x) - f_{j+1/2} = S(x),
\]

with \( f_{j+1/2} = f(x_{j+1/2}) \). Using the definition of \( A \) in (4.2) and the first property in (4.6), it is clear that the flux vector can be rewritten as

\[
f = -E e^{xA} \left(e^{-xA} \varphi\right)'.
\]

Next, combining this expression with (4.7), integrating from \( x_j \) to \( x_{j+1} \) and using the first three properties in (4.6) we obtain the following relation for the flux

\[
\int_{x_j}^{x_{j+1}} e^{-xA} dx \ E^{-1} f_{j+1/2} = e^{-x_j A} \varphi_j - e^{-x_{j+1} A} \varphi_{j+1} - \int_{x_j}^{x_{j+1}} e^{-xA} E^{-1} S \ dx.
\]

Consider the computation of the integral in the left hand side of (4.9). The difficulty is that \( A \) might be singular, in case \( U \) is singular. Using the spectral decomposition (4.4) we can compute the integral as follows

\[
\int_{x_j}^{x_{j+1}} e^{-xA} dx = V \int_{x_j}^{x_{j+1}} e^{-xA} dx \ V^{-1},
\]

\[
\int_{x_j}^{x_{j+1}} e^{-xA} dx = \text{diag} \left( \int_{x_j}^{x_{j+1}} e^{-xA_i} dx \right).
\]
When $A$ is singular, at least one of its eigenvalues $\lambda_i = 0$. Taking this into consideration the integrals in the right hand side of (4.10b) have to be formulated as
\[
\int_{x_j}^{x_{j+1}} e^{-\lambda_i x} \, dx = \Delta x \, e^{-\lambda_i x_{j+1}/2} \sinh\left(\frac{1}{2} \lambda_i \Delta x\right),
\]  
(4.11)
where the function $\sinh c$ is defined as $\sinh c(z) = \sinh z / z$ for $z \neq 0$ and $\sinh c(0) = 1$, and therefore (4.11) is correct for both $\lambda_i \neq 0$ and $\lambda_i = 0$. Substituting (4.11) in (4.10) and using the definition of matrix functions in (4.5) the integral of $e^{-x A}$ can be evaluated as
\[
\int_{x_j}^{x_{j+1}} e^{-x A} \, dx = \Delta x \, e^{-x_{j+1}/2 A} \sinh\left(\frac{1}{2} P\right).
\]  
(4.12)
Finally, inserting this relation in the left hand side of (4.9), we can derive the following expression for the flux
\[
f_{j+1/2} = \frac{1}{\Delta x} \mathcal{E} \left( \sinh c\left(\frac{1}{2} P\right) \right)^{-1} e^{x_j/2 A} \left( e^{-x_j A} \varphi_j - e^{-x_{j+1} A} \varphi_{j+1} - \int_{x_j}^{x_{j+1}} e^{-x A} \mathcal{E}^{-1} S \, dx \right),
\]  
(4.13)
thus also in the system case the flux is a superposition of a homogeneous and an inhomogeneous component, as anticipated. Note that $\sinh c\left(\frac{1}{2} P\right)$ is regular, even if $P$ is singular.

Consider first the homogeneous flux, which follows from (4.9) if we set $S(x) = 0$. Using the last property in (4.6) we can rewrite the expression for the homogeneous flux as
\[
f_{j+1/2}^{(h)} = \frac{1}{\Delta x} \mathcal{E} \left( B(-P) \varphi_j - B(P) \varphi_{j+1} \right),
\]  
(4.14)
analogous to the scalar flux; cf. (3.4a). For the numerical flux $F_{j+1/2}$ we simply take $F_{j+1/2}^{(h)} = f_{j+1/2}^{(h)}$.

Rearranging terms in (4.14) and using the relation $B(-z) - B(z) = z$, we can derive the alternative representation
\[
F_{j+1/2}^{(h)} = \frac{1}{2} U (\varphi_j + \varphi_{j+1}) - \frac{1}{\Delta x} \frac{1}{2} \mathcal{E} \left( B(P) + B(-P) \right) (\varphi_{j+1} - \varphi_j),
\]  
(4.15)
reminiscent of the central difference approximation of (2.2), albeit with a modified diffusion matrix $\frac{1}{2} \mathcal{E} \left( B(P) + B(-P) \right)$.

The derivation of the inhomogeneous flux is more involved. Substituting the expression for $S(x)$ in the integral in (4.13) and changing the order of integration, we obtain
\[
f_{j+1/2}^{(i)} = -\frac{1}{\Delta x} \mathcal{E} \left( \sinh c\left(\frac{1}{2} P\right) \right)^{-1} \int_{x_j}^{x_{j+1}} \int_{x}^{x_{\text{int}(x)}} e^{(x_{j+1}/2 - \xi) A} \, d\xi \, \mathcal{E}^{-1} S(x) \, d\xi,
\]  
(4.16)
where $x_{\text{int}(x)} = x_j$ for $x_j \leq x \leq x_{j+1}/2$ and $x_{\text{int}(x)} = x_{j+1}$ for $x_{j+1}/2 < x \leq x_{j+1}$, i.e., the $x$-coordinate of the interface closest to $x$. Introducing the scaled coordinate $\sigma(x) = (x - x_j) / \Delta x$, we can derive the following alternative expression for the inhomogeneous flux
\[
f_{j+1/2}^{(i)} = \Delta x \mathcal{E} \int_{0}^{1} G(\sigma; P) \mathcal{E}^{-1} S(x(\sigma)) \, d\sigma;
\]  
(4.17)
Numerical Approximation of the Flux Vector

from (3.4b). The matrix $G$ in (4.17), relating the flux vector to the source term vector, is referred to as the Green’s matrix for the flux and is given by

$$ G(\sigma; P) = \begin{cases} \sigma B(-\sigma P)B(-\sigma P)^{-1} & \text{for } 0 \leq \sigma \leq \frac{1}{2}, \\ -(1-\sigma)B(\sigma P)B((1-\sigma)P)^{-1} & \text{for } \frac{1}{2} < \sigma \leq 1. \end{cases} \quad (4.18a) $$

Note that the matrices $B(-\sigma P)$ and $B((1-\sigma)P)$ are always regular. When the Peclet matrix $P$ is nonsingular, this expression reduces to

$$ G(\sigma; P) = \begin{cases} \left( I - e^{-P}\right)^{-1} \left( I - e^{-\sigma P}\right) & \text{for } 0 \leq \sigma \leq \frac{1}{2}, \\ -\left( I - e^{P}\right)^{-1} \left( I - e^{(1-\sigma)P}\right) & \text{for } \frac{1}{2} < \sigma \leq 1; \end{cases} \quad (4.18b) $$

cf. (3.5). In the derivation of (4.18b) we used that $P$ commutes with $g(P)$ for arbitrary $g$. This matrix satisfies the relation $G(\frac{1}{2}; P) - G(\frac{1}{2}+; P) = I$, implying that the diagonal entries are discontinuous at $\sigma = \frac{1}{2}$ with jump 1, whereas the off-diagonal entries are continuous. By analogy with the scalar case, we replace in the integral representation (4.17) the source term $s(x(\sigma))$ by its upwind value $s_{u,j+1/2}$, to be specified shortly, and evaluate the resulting integral exactly, to obtain the inhomogeneous numerical flux

$$ F_{j+1/2}^{(i)} = \Delta x \left( \frac{1}{2} I - \mathcal{E}W(P)\mathcal{E}^{-1} \right) s_{u,j+1/2}, \quad (4.19) $$

with $W(P)$ defined in (4.5) with $g(z) = W(z)$. Note that the matrices $\mathcal{E}$ and $\mathcal{E}^{-1}$ do not cancel out, unless the matrices $U$ and $\mathcal{E}$ commute.

The upwind value of $s$ is not trivial since different advection velocities are intertwined. Therefore, we first decouple system (4.1a) as follows

$$ \mathbf{L} \psi' - \psi'' = (\mathcal{E}V)^{-1}s =: \tilde{s}, \quad (4.20a) $$

where $\psi = V^{-1}\varphi$, or written componentwise

$$ \lambda_i \psi_i' - \psi_i'' = \tilde{s}_i, \quad (i = 1, 2, \ldots, m). \quad (4.20b) $$

From these scalar advection-diffusion-reaction equations for $\psi_i$ we conclude that the upwind values for $\tilde{s}_i$ are $\tilde{s}_{i,\text{u},j+1/2} = \tilde{s}_{i,j}$ if $\lambda_i \geq 0$ and $\tilde{s}_{i,\text{u},j+1/2} = \tilde{s}_{i,j+1}$ if $\lambda_i < 0$, or alternatively,

$$ \tilde{s}_{i,\text{u},j+1/2} = \frac{1}{2} \left( 1 + \text{sgn}(\lambda_i) \right) \tilde{s}_{i,j} + \frac{1}{2} \left( 1 - \text{sgn}(\lambda_i) \right) \tilde{s}_{i,j+1}. \quad (4.21) $$

Combining these relations in vector form, using the definition of $\text{sgn}(A)$ in (4.5), we have

$$ \tilde{s}_{u,j+1/2} = \frac{1}{2} (I + \text{sgn}(A)) \tilde{s}_j + \frac{1}{2} (I - \text{sgn}(A)) \tilde{s}_{j+1}. \quad (4.22) $$

The upwind value of $s$ is then given by $s_{u,j+1/2} = \mathcal{E}V\tilde{s}_{u,j+1/2}$, which can be expressed in terms of $s_j$ and $s_{j+1}$ as follows

$$ s_{u,j+1/2} = \frac{1}{2} (I + \sigma) s_j + \frac{1}{2} (I - \sigma) s_{j+1} \quad \sigma = \mathcal{E}\text{sgn}(A)\mathcal{E}^{-1}, \quad (4.23) $$

with the matrix sign function $\text{sgn}(A)$ defined in (4.5).

To summarize, the numerical flux $F_{j+1/2}$ is the superposition

$$ F_{j+1/2} = F_{\text{h}}_{j+1/2}^{(h)} + F_{\text{h}}^{(i)}_{j+1/2}, \quad (4.24) $$

with the homogeneous component $F_{\text{h}}^{(h)}_{j+1/2} = f_{\text{h}}^{(h)}_{j+1/2}$ defined in (4.14) and the inhomogeneous component $F_{\text{h}}^{(i)}_{j+1/2}$ defined in (4.19) and (4.23). This flux approximation is referred to as the complete flux (CF) scheme for systems.
5 Elaboration of the scheme

We give the final discretisation scheme for (2.1). Moreover, we elaborate the scheme for a model problem and investigate its behaviour for a few limiting cases, i.e., dominant advection or diffusion and/or strong or weak coupling.

To derive the final scheme, we combine the discrete conservation law (2.4) with the complete flux approximation. This way we obtain

\[-\alpha \varphi_{j-1} + (\alpha + \beta) \varphi_j - \beta \varphi_{j+1} = \Delta x (\gamma s_{j-1} + (I - \gamma + \delta)s_j - \delta s_{j+1}),\]

referred to as the finite volume-complete flux (FV-CF) scheme, where the coefficient matrices \( \alpha \) etc. are defined by

\[
\alpha = \frac{1}{\Delta x} E B(-P), \quad \beta = \frac{1}{\Delta x} E B(P), \\
\gamma = \frac{1}{2} Q(I + \sigma), \quad \delta = \frac{1}{2} Q(I - \sigma), \quad Q = \frac{1}{2} I - E W(P)E^{-1}.
\]

The FV-CF scheme has a three-point coupling for both \( \varphi \) and \( s \), the latter due to the inclusion of the inhomogeneous flux. In Section 6 we compare the CF scheme for the flux approximation with the homogeneous flux (HF) scheme, which only includes the homogeneous component (4.14). This means that \( \gamma = \delta = 0 \) in (5.1).

It is instructive to apply the CF scheme to a model problem for which

\[
U = \begin{pmatrix} -u & 0 \\ 0 & u \end{pmatrix}, \quad E = \frac{1}{2 \varepsilon} \begin{pmatrix} 1 + \alpha & 1 - \alpha \\ 1 - \alpha & 1 + \alpha \end{pmatrix},
\]

thus there are two advection velocities involved, viz. \( u_1 = -u < 0 \) and \( u_2 = u > 0 \) and \( E \) is symmetric positive definite with eigenvalues \( \varepsilon \) and \( \varepsilon \alpha \) and corresponding orthogonal eigenvectors \((1, 1)^T\) and \((-1, 1)^T\), respectively. The parameter \( \alpha \), \( 0 < \alpha \leq 1 \) determines the coupling between the constituting equations; for \( \alpha \ll 1 \) the coupling is strong and for \( \alpha = 1 \) the system is decoupled. The corresponding matrix \( A \) is given by

\[
A = \frac{u}{2 \varepsilon \alpha} \begin{pmatrix} -1 - \alpha & -1 + \alpha \\ 1 - \alpha & 1 + \alpha \end{pmatrix},
\]

with eigenvalues and eigenvectors given by

\[
\Lambda = \frac{u}{\varepsilon \sqrt{\alpha}} \text{diag}(-1, 1), \quad V = \begin{pmatrix} 1 + \sqrt{\alpha} & -1 + \sqrt{\alpha} \\ -1 + \sqrt{\alpha} & 1 + \sqrt{\alpha} \end{pmatrix}.
\]

Note that the eigenvectors of \( A \) are not orthogonal, unless \( \alpha = 1 \).

In order to determine the numerical fluxes, we need the matrix functions \( B(\pm P) \), \( W(P) \) and \( \text{sgn}(A) \). Applying the definition of a matrix function in (4.5) and using the relations \( B(z) = \frac{1}{2}(B(z) + B(-z)) - \frac{1}{2} z \) and \( W(z) + W(-z) = 1 \), we obtain

\[
B(\pm P) = \frac{1}{2}(B^+ + B^-) I + \frac{1}{2} P, \quad B^\pm = B(\pm p/\sqrt{\alpha}), \\
W(P) = \frac{1}{2} I + \frac{1 - 2W^+}{4 \sqrt{\alpha}} \begin{pmatrix} 1 + \alpha & 1 - \alpha \\ -1 + \alpha & -1 - \alpha \end{pmatrix} = \frac{1}{2} I + \frac{W^+ - \frac{1}{2} p}{p/\sqrt{\alpha}} P, \quad W^+ = W(p/\sqrt{\alpha}),
\]

(5.6a)

(5.6b)
5 ELABORATION OF THE SCHEME

where \( p = u \Delta x / \varepsilon \) is a (scalar) Peclet number; cf. (3.2). Let \( B(P) = (b_{ij}(p)) \) and \( W(P) = (w_{ij}(p)) \), then the matrix elements satisfy the relations \( b_{21}(p) = -b_{12}(p) \), \( b_{22}(p) = b_{11}(-p) \), \( w_{21}(p) = -w_{12}(p) \) and \( w_{11}(p) + w_{22}(p) = 1 \). Elements of the matrix functions \( B(P) \) and \( W(P) \) for several values of \( \alpha \) are plotted in Figure 3 and 4, respectively. Note that for \( \alpha = 1 \), i.e., for a decoupled system, \( b_{11}(p) = B(-p) \), \( b_{12}(p) = 0 \), and consequently, the flux component \( f_{1,j+1/2}^{(h)} \) reduces to the scalar flux (3.4a). Likewise, \( w_{11}(p) = W(-P) \) and \( w_{12}(p) = 0 \) for \( \alpha = 1 \), and \( f_{1,j+1/2}^{(i)} \) is just the scalar inhomogeneous flux in (3.6). For decreasing \( \alpha \), the off-diagonal elements \( b_{12}(p) \) and \( w_{12}(p) \) become increasingly more important. Moreover, from Figure 4 it is clear that for small \( |p| \), i.e. dominant diffusion, \( w_{11}(p) - \frac{1}{2} \) and \( w_{12}(p) \) are small, and consequently, the inhomogeneous flux is of little importance; cf. (4.19). On the other hand, for dominant advection characterised by large \( |p| \), the inhomogeneous flux is significant. For \( \text{sgn}(A) \) and the corresponding matrix \( \sigma \) we have

\[
\text{sgn}(A) = \frac{1}{2 \sqrt{\alpha}} \begin{pmatrix} -1 - \alpha & -1 + \alpha \\ 1 - \alpha & 1 + \alpha \end{pmatrix} = \frac{\varepsilon \sqrt{\alpha}}{u} A, \quad \sigma = \frac{1}{2 \sqrt{\alpha}} \begin{pmatrix} -1 - \alpha & 1 - \alpha \\ -1 + \alpha & 1 + \alpha \end{pmatrix}.
\]  

(5.7)

Note that these matrices satisfy \( \text{sgn}(A)^2 = \sigma^2 = I \).
Using (5.6) and (5.7), we can derive the following expressions for the numerical flux

\[ F_{j+1/2}^{(h)} = \frac{1}{2} U (\varphi_j + \varphi_{j+1}) - \frac{1}{\Delta x} \frac{1}{2} (B^+ + B^-) E (\varphi_{j+1} - \varphi_j), \]  

(5.8a)

\[ F_{j+1/2}^{(i)} = \Delta x \frac{1}{2} \frac{W^+}{2 \sqrt{\alpha}} \begin{pmatrix} -1 - \alpha & 1 - \alpha \\ -1 + \alpha & 1 + \alpha \end{pmatrix} s_{u,j+1/2}, \]  

(5.8b)

with \( s_{u,j+1/2} \) defined in (4.23). Next, we consider a few limit cases. First, consider \( p \to 0 \), i.e., diffusion is dominant, then \( \frac{1}{2} (B^+ + B^-) \to 1 \), and consequently, the homogeneous flux in (5.8) reduces to the central difference approximation. Moreover \( W^+ \to \frac{1}{2} \), implying that the inhomogeneous flux is negligible. Second, consider the limit \( p \to \infty \) with \( \varepsilon p = \text{Const} \). Then the homogeneous flux reduces to the advective flux

\[ F_{j+1/2}^{(h)} = \frac{u}{4 \sqrt{\alpha}} \begin{pmatrix} (1 - \sqrt{\alpha})^2 & 1 - \alpha \\ 1 - \alpha & (1 + \sqrt{\alpha})^2 \end{pmatrix} \varphi_j - \frac{u}{4 \sqrt{\alpha}} \begin{pmatrix} (1 + \sqrt{\alpha})^2 & 1 - \alpha \\ 1 - \alpha & (1 - \sqrt{\alpha})^2 \end{pmatrix} \varphi_{j+1}, \]  

(5.9)

where the components are still coupled. The inhomogeneous flux is still defined by (5.8b), with \( W^+ = 0 \). Finally, we take in addition \( \alpha \to 1 \), which means that the equations decouple. In this case we have

\[ F_{j+1/2}^{(h)} = u \begin{pmatrix} -\varphi_1,j+1 & \varphi_2,j \end{pmatrix}, \quad F_{j+1/2}^{(i)} = \frac{1}{2} \Delta x \begin{pmatrix} -s_1,j+1 \\ s_2,j \end{pmatrix}, \]  

(5.10)

i.e., \( F_{j+1/2}^{(h)} \) is the upwind approximation of the advective flux \( f_{ad} = u (-\varphi_1, \varphi_2)^T \). Substituting the various approximations of the flux in the discrete conservation law then gives the final scheme.

### 6 Numerical example

In this section we apply the CF and HF schemes to a model problem to assess their (order of) accuracy. We consider only advection-dominated flow, for both a weakly and a strongly coupled system.

**Example** Advection-diffusion-reaction system with interior layer.

We solve the BVP

\[
(U \varphi - E \varphi')' = s, \quad 0 < x < 1, \\
\varphi_1(0) = 0, \quad \varphi_1(1) = \varphi_{1,R}, \quad \varphi_2(0) = \varphi_{2,L}, \quad \varphi_2(1) = 0,
\]

(6.1a)

(6.1b)

where the advection and the diffusion matrices \( U \) and \( E \) and the source term \( s \) are given by

\[
U = \begin{pmatrix} u_1 & 0 \\ 0 & u_2 \end{pmatrix}, \quad E = \frac{1}{2} \varepsilon \begin{pmatrix} 1 + \alpha & 1 - \alpha \\ 1 - \alpha & 1 + \alpha \end{pmatrix}, \quad s(x) = \frac{s_{\max}}{1 + s_{\max}^2 (2x - 1)^2} \begin{pmatrix} 1 \\ 0.2 \end{pmatrix},
\]

(6.2)

respectively. We take \( u_1 < 0 \) and \( u_2 > 0 \) in agreement with the boundary conditions in (6.1b), i.e., \( x = 1 \) is the inflow and \( x = 0 \) the outflow boundary for \( \varphi_1 \), corresponding to the Dirichlet and Neumann boundary condition, respectively, and vice versa for \( \varphi_2 \). The diffusion matrix \( E \) is the same as in (5.3). The source term has a sharp peak at \( x = \frac{1}{2} \), causing a steep interior layer, provided \( 0 < \varepsilon \ll 1 \). Typical solutions of (6.1) are shown in Figure 5.
7 Summary, Conclusions and Future Research

In order to handle the combination of Dirichlet and Neumann boundary conditions, say at \( x = 0 \), we require the difference equation (5.1) to hold at the first grid point \( x_1 = 0 \), thus introducing the unknown \( \varphi_0 \) in the virtual grid point \( x_0 = -\Delta x \). We have to eliminate \( \varphi_0 \) using the boundary conditions at \( x = 0 \). Applying the standard central difference approximation to \( \varphi_1'(0) = 0 \) and linear extrapolation to \( \varphi_2 \), we obtain the second order approximations \( \varphi_1,0 = \varphi_{1,2} \) and \( \varphi_2,0 = 2\varphi_{2,L} - \varphi_{2,2} \), or written in matrix-vector form,

\[
\varphi_0 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \varphi_2 + 2\varphi_{2,L} \begin{pmatrix} 0 \\ 1 \end{pmatrix} .
\]

The boundary conditions at \( x = 1 \) are treated in a similar way.

We consider the CF and HF numerical solutions for \( \varepsilon = 10^{-8} \), i.e., advection dominated flow. In this case it is meaningful to compare the numerical solutions with the reduced solution \( \varphi_r \) of (6.1), i.e., the solution with \( \mathcal{E} = O \) and omitting the Neumann outflow boundary conditions. Let \( h = \Delta x \) be the grid size. To determine the accuracy of a numerical solution we compute the average errors \( e_{i,h} := ||\varphi_i - \varphi_{r,i}||_1/N (i = 1, 2) \), where \( \varphi_{r,i} \) denotes the \( i \)th component of the reduced solution restricted to the grid. Figure 6 shows \( e_{i,h} \) as a function of \( h \) for \( \alpha = 0.05 \) (strong coupling) and \( \alpha = 0.75 \) (weak coupling). From this figure it is clear that initially, on rather coarse grids, discretisation errors of both flux approximations are of the same order, whereas for decreasing \( h \) the CF scheme tends to become more accurate. In fact, the HF approximation reduces to first order convergence, in agreement with the observation that the HF flux is just the upwind flux for pure advection-reaction problems. On the other hand, the CF flux approximation seems to have a higher order of convergence.

7 Summary, conclusions and future research

We have extended the complete flux scheme to steady, one-dimensional advection-diffusion-reaction systems, including the coupling between the constituent equations in the (space)discretization. Moreover, we restrict ourselves to constant-coefficient systems, i.e., the advection and diffusion matrices are assumed to be constant. This is not a severe restriction, since for nonconstant coefficient matrices we
can easily extend the scheme by taking a piecewise constant approximation of the advection and diffusion matrices. To derive the scheme, we first determine an integral representation for the flux vector from a local system BVP for the entire system, including the source term vector. As a result, the flux vector consists of two parts, i.e., a homogeneous and an inhomogeneous flux, corresponding to the advection-diffusion operator and the source term vector, respectively. An alternative expression of the inhomogeneous flux in terms of the so-called Green’s matrix is given. Next, replacing the source term vector by its upwind value, we could derive the numerical flux, which obviously is also a superposition of a homogeneous and inhomogeneous part. The numerical flux is almost identical to its scalar counterpart, the major difference is that the Peclet number $P$ should be replaced by the Peclet matrix $P = (p_{ij})$ and the functions operating on $P$ should be replaced by their matrix versions.

The inclusion of the inhomogeneous flux is very important for dominant advection, since it ensures that the flux approximation remains second order accurate, in contrast to the homogeneous flux which reduces to the upwind flux when $p_{ij} \to \infty$. The resulting finite volume-complete flux scheme displays second order convergence when the grid size $\Delta x \to 0$, even for very large $p_{ij}$, never generates spurious oscillations, and has a three-point coupling, resulting in a block-tridiagonal system.

Extensions of the scheme we have in mind are the following. First, extension to time dependent problems is very important. Following the approach in [14], we will include the time-derivative in the inhomogeneous flux, resulting in a semi-implicit ODE-system. For scalar equations this approach turned out to be very benificial resulting in very small dissipation and dispersion errors. Second, extension to two and three-dimensional problems is required; see [15] where the two-dimensional scalar scheme is discussed. Finally, we will apply the scheme to more realistic problems from continuum physics, like the simulation of plasmas or laminar flames governed by multi-species diffusion. A first effort in this direction is presented in [8, 2] where the homogeneous flux approximation is applied to the numerical simulation of plasmas.

References

REFERENCES


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