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Abstract We consider the complete flux (CF) scheme, a finite volume method (FVM) presented in [3]. CF is based on an integral representation for the fluxes, found by solving a local boundary value problem that includes the source term. It performs well (second order accuracy) for both diffusion and advection dominated problems. In this paper we focus on cylindrically symmetric conservation laws of advection-diffusion-reaction type.

1 Introduction

We consider a stationary conservation law of advection-diffusion-reaction type, viz.

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

where $\mathbf{u}$ is a mass flux or (drift) velocity, $\varepsilon \geq \varepsilon_{\min} > 0$ a diffusion coefficient, and s a source term describing, e.g., chemical reactions or ionization. The unknown φ is then the mass fraction of one of the constituent species in a chemically reacting flow or a plasma [2]. The parameters ε and s are usually (complicated) functions of φ whereas the vector field $\mathbf{u}$ has to be computed from (flow) equations corresponding to (1). However, for the sake of discretization, we will consider these parameters as given functions of the spatial coordinates.

Associated with equation (1) we introduce the flux vector $\mathbf{f}$, defined by $\mathbf{f} := \mathbf{u}\varphi - \varepsilon\nabla\varphi$. Consequently, equation (1) can be concisely written as $\nabla\cdot\mathbf{f} = s$. Integrating this equation over a fixed domain Ω and applying Gauss's theorem we obtain the integral form of the conservation law, i.e.,

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$$\oint_{\Gamma} (\mathbf{f},\mathbf{n})\, dS = \int_{\Omega} s\, dV, \tag{2}$$

where $\mathbf{n}$ is the outward unit normal on the boundary $\Gamma = \partial\Omega$. In the FVM [1] we cover the domain with a finite number of disjunct control volumes or cells and impose the integral form (2) for each of these cells.

For cylindrical coordinates (r,θ,z), we assume cylindrical symmetry, i.e., $\varphi = \varphi(r,z)$ and $\mathbf{f} = f_r(r,z)\mathbf{e}_r + f_z(r,z)\mathbf{e}_z$. Equation (1) becomes

$$\frac{1}{r}\frac{\partial}{\partial r}(rf_r) + \frac{\partial}{\partial z}(f_z) = \frac{1}{r}\frac{\partial}{\partial r}\left(r\left(u_r\varphi - \varepsilon\frac{\partial\varphi}{\partial r}\right)\right) + \frac{\partial}{\partial z}\left(u_z\varphi - \varepsilon\frac{\partial\varphi}{\partial z}\right) = s. \tag{3}$$

We choose a uniform tensor product grid with coordinates (r_i, z_j) and grid spacings Δr and Δz. A control volume is the cylindrical shell $\Omega_{i,j} = [r_{i-\frac{1}{2}}, r_{i+\frac{1}{2}}] \times [0, 2\pi) \times [z_{j-\frac{1}{2}}, z_{j+\frac{1}{2}}]$. The surface integral of the flux over the boundary $\Gamma_{i,j} = \partial\Omega_{i,j}$ contains four terms and is given by

$$\oint_{\Gamma_{i,j}} (\mathbf{f},\mathbf{n})\, dS = \int_{r=r_{i+\frac{1}{2}}} f_r\, dS - \int_{r=r_{i-\frac{1}{2}}} f_r\, dS + \int_{z=z_{j+\frac{1}{2}}} f_z\, dS - \int_{z=z_{j-\frac{1}{2}}} f_z\, dS, \tag{4}$$

where for example $r = r_{i+\frac{1}{2}}$ denotes the interface $\{r_{i+\frac{1}{2}}\} \times \left[0, 2\pi\right) \times \left[z_{j-\frac{1}{2}}, z_{j+\frac{1}{2}}\right]$, and likewise for all other interfaces. All integrals on the right hand side are approximated by the midpoint rule. Taking (2) for $\Omega = \Omega_{i,j}$ and approximating the volume integral for s with the midpoint rule too, we obtain the discrete conservation law

$$\left(r_{i+\frac{1}{2}} F_{r,i+\frac{1}{2},j} - r_{i-\frac{1}{2}} F_{r,i-\frac{1}{2},j}\right)\Delta z + r_i\left(F_{z,i,j+\frac{1}{2}} - F_{z,i,j-\frac{1}{2}}\right)\Delta r = r_i\, s_{i,j}\, \Delta r\, \Delta z, \tag{5}$$

where $F_{r,i+\frac{1}{2},j}$ is the numerical flux approximating $f_r(r_{i+\frac{1}{2}}, z_j)$ and likewise for $F_{z,i,j+\frac{1}{2}}$. The FVM has to be completed with expressions for the numerical flux. The derivation of expressions for the numerical flux is detailed in the next sections.

2 Integral representation of the flux

In this section we derive the r-component of the flux in *polar* coordinates by solving a local one-dimensional problem. To determine an integral relation for the flux $f_r := u_r\varphi - \varepsilon\frac{d\varphi}{dr}$ at $r = r_{i+\frac{1}{2}}$, we consider the one-dimensional model BVP:

$$\frac{d}{dr}(rf_r) = rs, \quad r_i < r < r_{i+1}, \qquad \varphi(r_i) = \varphi_i, \quad \varphi(r_{i+1}) = \varphi_{i+1}. \tag{6}$$

We assume $u_r \neq 0$, $\varepsilon > 0$ and s to be sufficiently smooth functions of r.

We introduce the variables U, D, a, A and S by

$$U := ru_r, \quad D := \varepsilon r, \quad a := \frac{U}{D}, \quad A := \int_{r_{i+\frac{1}{2}}}^{r} a(\rho)\,d\rho, \quad S := \int_{r_{i+\frac{1}{2}}}^{r} \rho\, s(\rho)\,d\rho, \tag{7}$$

and integrate (6) from the cell boundary $r_{i+\frac{1}{2}}$ to $r \in (r_i, r_{i+1})$ to find the integral relation $rf_r - (rf_r)_{i+\frac{1}{2}} = S$. Then we rewrite the flux in terms of its integrating factor, viz. $f_r = -\varepsilon\, \mathrm{e}^{A}\, \frac{d}{dr}\left(\mathrm{e}^{-A}\,\varphi\right)$, substitute it in the integral relation and subsequently integrate over the interval (r_i, r_{i+1}), to arrive at the following expression

$$(rf_r)_{i+\frac{1}{2}} = \underbrace{\frac{\mathrm{e}^{-A_i}\varphi_i - \mathrm{e}^{-A_{i+1}}\varphi_{i+1}}{\langle D^{-1}, \mathrm{e}^{-A}\rangle}}_{(rf_r^{\mathrm{hom}})_{i+\frac{1}{2}}} \underbrace{- \frac{\langle D^{-1}S, \mathrm{e}^{-A}\rangle}{\langle D^{-1}, \mathrm{e}^{-A}\rangle}}_{(rf_r^{\mathrm{inh}})_{i+\frac{1}{2}}}. \tag{8}$$

Here we have used the inner product $\langle f, g\rangle := \int_{r_i}^{r_{i+1}} fg\,dr$. In (8) we have introduced the homogeneous flux f_r^{hom} and the inhomogeneous flux f_r^{inh}. Note that the fluxes correspond to the advection-diffusion operator and the source term, respectively.

Using $A' = a$, we find by straightforward evaluation $\langle a, \mathrm{e}^{-A}\rangle = \mathrm{e}^{-A_i} - \mathrm{e}^{-A_{i+1}}$ and $\langle a, 1\rangle = A_{i+1} - A_i$. Now, we can write the homogeneous flux as

$$(rf_r^{\mathrm{hom}})_{i+\frac{1}{2}} = \frac{\langle a, \mathrm{e}^{-A}\rangle / \langle a, 1\rangle}{\langle D^{-1}, \mathrm{e}^{-A}\rangle} \Big(B\big(-\langle a, 1\rangle\big)\varphi_i - B\big(\langle a, 1\rangle\big)\varphi_{i+1}\Big), \tag{9}$$

with $B(x) := \frac{x}{\mathrm{e}^x - 1}$. Note that expression (9) for the homogeneous flux is exact. No approximations have been made so far. If both U and ε are constant, we have

$$A = \frac{U}{\varepsilon} \ln\left(\frac{r}{r_{i+\frac{1}{2}}}\right), \quad \langle a, 1\rangle = \frac{U}{\varepsilon} \ln\left(\frac{r_{i+1}}{r_i}\right), \quad \langle D^{-1}, \mathrm{e}^{-A}\rangle = \frac{1}{U}\langle a, \mathrm{e}^{-A}\rangle, \tag{10}$$

and (9) reduces to the *constant coefficient flux*

$$(rf_r^{\mathrm{hom}})_{i+\frac{1}{2}} = \frac{\varepsilon}{\ln(r_{i+1}/r_i)} \Big(B(-P)\varphi_i - B(P)\varphi_{i+1}\Big), \quad P := \frac{U}{\varepsilon} \ln\left(\frac{r_{i+1}}{r_i}\right). \tag{11}$$

Here we have introduced the Péclet number P.

Let us now consider the inhomogeneous flux. We first consider the general case, so nonconstant U and ε. The denominator in (8) for $\left(rf^{\mathrm{inh}}\right)_{i+\frac{1}{2}}$ can be written as

$$\langle D^{-1}, \mathrm{e}^{-A}\rangle = \langle \frac{a}{U}, \mathrm{e}^{-A}\rangle = \frac{1}{U^*}\langle a, \mathrm{e}^{-A}\rangle = -\frac{1}{U^*}\mathrm{e}^{-A_i}\left(\mathrm{e}^{-\langle a,1\rangle} - 1\right), \tag{12}$$

where $U^* = U(\xi)$ for some unknown $\xi \in (r_i, r_{i+1})$. For the numerator in (8), we substitute the expression for S and change the order of integration, viz.

$$\langle D^{-1}S, \mathrm{e}^{-A}\rangle = -\int_{r_i}^{r_{i+\frac{1}{2}}}\int_{r_i}^{\rho} D(r)^{-1}\mathrm{e}^{-A(r)}\,dr\,\rho\,s(\rho)\,d\rho + \int_{r_{i+\frac{1}{2}}}^{r_{i+1}}\int_{\rho}^{r_{i+1}} D(r)^{-1}\mathrm{e}^{-A(r)}\,dr\,\rho\,s(\rho)\,d\rho. \tag{13}$$

Carrying out the inner integrations over r, analogous to (12), we have

$$\left(rf_r^{\mathrm{inh}}\right)_{i+\frac{1}{2}} = \frac{U^*}{U_1^*}\int_{r_i}^{r_{i+\frac{1}{2}}} \frac{\mathrm{e}^{-\int_{r_i}^{\rho} a\,dr}-1}{\mathrm{e}^{-\langle a,1\rangle}-1}\rho\,s(\rho)\,d\rho - \frac{U^*}{U_2^*}\int_{r_{i+\frac{1}{2}}}^{r_{i+1}} \frac{\mathrm{e}^{-\int_{\rho}^{r_{i+1}} a\,dr}-1}{\mathrm{e}^{\langle a,1\rangle}-1}\rho\,s(\rho)\,d\rho, \tag{14}$$

with $U_1^* = U(\xi_1)$ for some unknown $\xi_1 \in (r_i, r_{i+\frac{1}{2}})$ and $U_2^* = U(\xi_2)$ for some unknown $\xi_2 \in (r_{i+\frac{1}{2}}, r_{i+1})$. Let us consider again the constant coefficient case, so assume that both U and ε are constant. Expression (14) can be simplified by introducing the *normalized coordinate*

$$\sigma(r) := \frac{1}{\langle a,1\rangle}\int_{r_i}^{r} a\,d\rho, \qquad r_i \le r \le r_{i+1}. \tag{15}$$

For both positive and negative values of u_r (and hence a) on (r_i, r_{i+1}), we have $d\sigma/dr > 0$. Therefore the normalized coordinate is an increasing function of r. It satisfies $0 \le \sigma \le 1$. Next we define the *Green's function for the flux* by

$$G(\sigma;P) := \begin{cases} \dfrac{\mathrm{e}^{-\sigma P}-1}{\mathrm{e}^{-P}-1}, & \text{for } 0 \le \sigma \le \sigma(r_{i+\frac{1}{2}}), \\[2ex] -\dfrac{\mathrm{e}^{(1-\sigma)P}-1}{\mathrm{e}^{P}-1}, & \text{for } \sigma(r_{i+\frac{1}{2}}) < \sigma \le 1. \end{cases} \tag{16}$$

With (15) and (16), equation (14) simplifies to

$$\left(rf_r^{\mathrm{inh}}\right)_{i+\frac{1}{2}} = \int_0^1 G(\sigma;\langle a,1\rangle)\,r(\sigma)\,s(r(\sigma))\,\frac{\langle a,1\rangle}{a(r(\sigma))}\,d\sigma. \tag{17}$$

If $u_r = 0$ on (r_i, r_{i+1}), then also $a = P = 0$. In this case, we can define the normalized coefficient σ by replacing a with D^{-1} in (15). This leads to a similar expression as (17) and will give the same numerical flux.

3 Numerical flux

For the numerical fluxes, we take U and ε constant on each control volume, viz. $\overline{U}_{i+\frac{1}{2}} := (U_i + U_{i+1})/2$ and $\overline{\varepsilon}_{i+\frac{1}{2}} := (\varepsilon_i + \varepsilon_{i+1})/2$. We use (11) to find the following *numerical homogeneous flux*

$$\left(rF_r^{\mathrm{hom}}\right)_{i+\frac{1}{2}} = \alpha_{r,i+\frac{1}{2}}\varphi_i - \beta_{r,i+\frac{1}{2}}\varphi_{i+1}, \tag{18a}$$

with

$$\alpha_{r,i+\frac{1}{2}} := B\big(-P_{r,i+\frac{1}{2}}\big)\frac{\overline{\varepsilon}_{i+\frac{1}{2}}}{\ln(r_{i+1}/r_i)}, \quad \beta_{r,i+\frac{1}{2}} := B\big(P_{r,i+\frac{1}{2}}\big)\frac{\overline{\varepsilon}_{i+\frac{1}{2}}}{\ln(r_{i+1}/r_i)},$$
$$P_{r,i+\frac{1}{2}} := \frac{\overline{U}_{i+\frac{1}{2}}}{\overline{\varepsilon}_{i+\frac{1}{2}}}\ln\left(\frac{r_{i+1}}{r_i}\right). \tag{18b}$$

The *numerical inhomogeneous flux* is based on (17). We make the approximation $\langle a,1\rangle/a(r(\sigma)) \doteq \Delta r$, and take $rs(r)$ equal to $r_i s_i$ on the interval $(0,\sigma(r_{i+\frac{1}{2}}))$ and equal to $r_{i+1}s_{i+1}$ on $(\sigma(r_{i+\frac{1}{2}}),1)$. Next we integrate the Green's function to find

$$\big(rF_r^{\text{inh}}\big)_{i+\frac{1}{2}} := \gamma_{r,i+\frac{1}{2}} s_i - \delta_{r,i+\frac{1}{2}} s_{i+1}, \tag{19a}$$

with

$$\gamma_{r,i+\frac{1}{2}} := r_i\Delta r\int_0^{\sigma_{i+\frac{1}{2}}} G(\sigma;P_{r,i+\frac{1}{2}})\,d\sigma = C(-P_{r,i+\frac{1}{2}};\sigma_{i+\frac{1}{2}})\,r_i\Delta r,$$
$$\delta_{r,i+\frac{1}{2}} := r_{i+1}\Delta r\int_{\sigma_{i+\frac{1}{2}}}^1 G(\sigma;P_{r,i+\frac{1}{2}})\,d\sigma = C(P_{r,i+\frac{1}{2}};1-\sigma_{i+\frac{1}{2}})\,r_{i+1}\Delta r,$$
$$\sigma_{i+\frac{1}{2}} := \frac{\ln(r_{i+\frac{1}{2}}/r_i)}{\ln(r_{i+1}/r_i)}, \qquad C(x;\sigma) := \frac{\mathrm{e}^{\sigma x}-1-\sigma x}{x\,(\mathrm{e}^x-1)}. \tag{19b}$$

It is easily verified that $\sigma_{i+\frac{1}{2}} \to \frac{1}{2}$ for $\Delta r \to 0$ when $r_i > 0$. The function C is plotted as a function of x for $\sigma = \frac{1}{2}$ in Figure 1. Note that $C(x;\sigma) \to \sigma^2/2$ for $x \to 0$, $C(x;\sigma) \to 0$ for $x \to \infty$, and finally $C(x;\sigma) \to \sigma$ for $x \to -\infty$. This means that for small Péclet numbers, the coefficients γ and δ will be approximately equal and the inhomogeneous flux is small. For large (positive or negative) Péclet numbers, the upwind value of s has a dominant contribution to the flux. This approach is similar to the modified inhomogeneous flux scheme for Cartesian coordinates in [2].

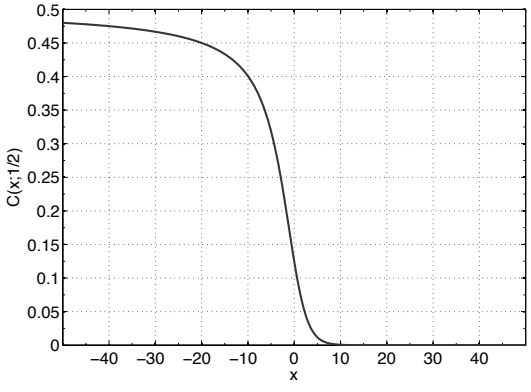

Fig. 1 Graph of the function $C(x;\sigma)$ as a function of x for $\sigma = \frac{1}{2}$. Note that $C(0;\frac{1}{2}) = \frac{1}{8}$, $C(x;\frac{1}{2}) \to 0$ for $x \to \infty$, and $C(x;\frac{1}{2}) \to \frac{1}{2}$ for $x \to -\infty$.

Adding (18) and (19), we obtain the following *numerical complete flux*:

$$\big(rF_r\big)_{i+\frac{1}{2}} = \alpha_{r,i+\frac{1}{2}}\varphi_i - \beta_{r,i+\frac{1}{2}}\varphi_{i+1} + \gamma_{r,i+\frac{1}{2}}s_i - \delta_{r,i+\frac{1}{2}}s_{i+1}. \tag{20}$$

4 Extension to two-dimensional conservation laws

Up till now we have considered the numerical flux for the r-component only (radial fluxes). The derivation of the flux in z-direction is similar. It is in fact the flux in Cartesian coordinates and a detailed derivation can be found in [3]. Here we only present the numerical flux. We have (cf. (18), (19), (20))

$$F_{z,j+\frac{1}{2}} = \alpha_{z,j+\frac{1}{2}}\varphi_j - \beta_{z,j+\frac{1}{2}}\varphi_{j+1} + \gamma_{z,j+\frac{1}{2}}s_j - \delta_{z,j+\frac{1}{2}}s_{j+1}, \tag{21a}$$

with

$$\alpha_{z,j+\frac{1}{2}} := B(-\overline{P}_{z,j+\frac{1}{2}})\frac{\widetilde{P}_{z,j+\frac{1}{2}}}{\overline{P}_{z,j+\frac{1}{2}}}\frac{\widetilde{\varepsilon}_{j+\frac{1}{2}}}{\Delta z}, \quad \beta_{z,j+\frac{1}{2}} := B(\overline{P}_{z,j+\frac{1}{2}})\frac{\widetilde{P}_{z,j+\frac{1}{2}}}{\overline{P}_{z,j+\frac{1}{2}}}\frac{\widetilde{\varepsilon}_{j+\frac{1}{2}}}{\Delta z},$$

$$\gamma_{z,j+\frac{1}{2}} := C(-\overline{P}_{z,j+\frac{1}{2}};\tfrac{1}{2})\Delta z, \quad \delta_{z,j+\frac{1}{2}} := C(\overline{P}_{z,j+\frac{1}{2}};\tfrac{1}{2})\Delta z, \quad P_z := \frac{u_z\Delta z}{\varepsilon}. \tag{21b}$$

Two averages are used in these expressions, the normal *arithmetic* mean $\overline{\varepsilon}_{j+\frac{1}{2}} := (\varepsilon_j+\varepsilon_{j+1})/2$ and a *weighted* average $\widetilde{\varepsilon}_{j+\frac{1}{2}} := W(-\overline{P}_{z,j+\frac{1}{2}})\varepsilon_j + W(\overline{P}_{z,j+\frac{1}{2}})\varepsilon_{j+1}$. The weight function used here is $W(x) := (\mathrm{e}^x - 1 - x)/(x(\mathrm{e}^x-1))$. Note that the expressions for the coefficients γ and δ in (21b) are different from those in [3]. These new coefficients coincide with the old for large Péclet numbers, but are more accurate if advection is not dominant.

We will now combine the one-dimensional schemes to derive a numerical scheme for the two-dimensional equation (1). For ease of presentation, we use both index notation and compass notation; see Figure 2. Thus, φ_{C} should be understood as $\varphi_{i,j}$ and $f_{r,\mathrm{e}}$ as $f_{r,i+\frac{1}{2},j}$ etc. The key idea is to include the cross flux term $\partial f_z/\partial z$ in the evaluation of the flux in r-direction. Therefore we determine the numerical flux $F_{r,i+\frac{1}{2},j}$ from the quasi-one-dimensional boundary value problem:

$$\frac{\partial}{\partial r}\Big(r\Big(u_r\varphi - \varepsilon\frac{\partial\varphi}{\partial r}\Big)\Big) = rs_r, \qquad r_i < r < r_{i+1}, z = z_j, \tag{22a}$$

$$\varphi(\mathbf{x}_{i,j}) = \varphi_{i,j}, \qquad \varphi(\mathbf{x}_{i+1,j}) = \varphi_{i+1,j}, \tag{22b}$$

where the modified source term s_r is defined by $s_r := s - \frac{\partial f_z}{\partial z}$. The derivation of the expression for the numerical flux is essentially the same as for (20), the main difference being the inclusion of the cross flux term $\partial f_z/\partial z$ in the source term. In the computation of s_r we replace $\partial f_z/\partial z$ by its central difference approximation and

for f_z we take the homogeneous numerical flux. A similar procedure applies to the z-component of the flux. This leads to the following algorithm.

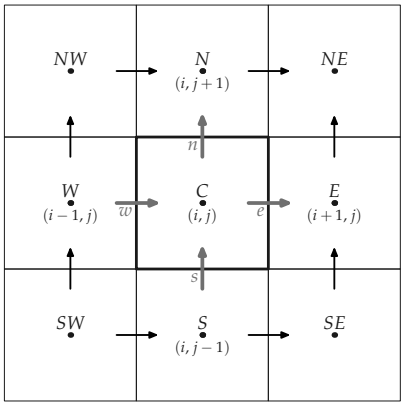

Fig. 2 Control volume Ω_C and corresponding stencil.

Algorithm for the computation of the numerical fluxes

1. Compute averages and Péclet numbers
   - in r-direction: $\overline{U}_e = \frac{U_C+U_E}{2}$, $\overline{\varepsilon}_e = \frac{\varepsilon_C+\varepsilon_E}{2}$, $P_{r,e} = \frac{\overline{U}_e}{\overline{\varepsilon}_e} \ln\left(\frac{r_E}{r_C}\right)$
   - in z-direction: $P_z = \frac{u_z \Delta z}{\varepsilon}$, $\overline{P}_{z,n} = \frac{P_{z,C}+P_{z,N}}{2}$, $\widetilde{\varepsilon}_n := W(-\overline{P}_{z,n})\varepsilon_C + W(\overline{P}_{z,n})\varepsilon_N$, $\widetilde{P}_{z,n} = W(-\overline{P}_{z,n})P_{z,C} + W(\overline{P}_{z,n})P_{z,N}$
2. Numerical homogeneous flux
   - in r-direction: $\left(rF_r^{\text{hom}}\right)_e = \alpha_{r,e}\varphi_C - \beta_{r,e}\varphi_E$ with $\alpha_{r,e} = B(-P_{r,e})\frac{\overline{\varepsilon}_e}{\ln(r_E/r_C)}$, $\beta_{r,e} = B(P_{r,e})\frac{\overline{\varepsilon}_e}{\ln(r_E/r_C)}$
   - in z-direction: $F_{z,n}^{\text{hom}} = \alpha_{z,n}\varphi_C - \beta_{z,n}\varphi_N$ with $\alpha_{z,n} = B(-\overline{P}_{z,n})\frac{\widetilde{P}_{z,n}}{\overline{P}_{z,n}}\frac{\widetilde{\varepsilon}_n}{\Delta z}$, $\beta_{z,n} = B(\overline{P}_{z,n})\frac{\widetilde{P}_{z,n}}{\overline{P}_{z,n}}\frac{\widetilde{\varepsilon}_n}{\Delta z}$
3. Numerical inhomogeneous flux
   - in r-direction: $\left(rF_r^{\text{inh}}\right)_e = \gamma_{r,e}s_{r,C} - \delta_{r,e}s_{r,E}$ with $\gamma_{r,e} = C\big(-P_{r,e};\sigma_e\big)\,r_C\,\Delta r$, $\delta_{r,e} = C\big(P_{r,e};1-\sigma_e\big)\,r_E\,\Delta r$, $\sigma_e = \frac{\ln(r_e/r_C)}{\ln(r_E/r_C)}$, $s_{r,C} = s_C - \frac{1}{\Delta z}\left(F_{z,n}^{\text{hom}} - F_{z,s}^{\text{hom}}\right)$
   - in z-direction: $F_{z,n}^{\text{inh}} = \gamma_{z,n}s_{z,C} - \delta_{z,n}s_{z,N}$ with $\gamma_{z,n} = C\big(-\overline{P}_{z,n};\frac{1}{2}\big)\,\Delta z$, $\delta_{z,n} = C\big(\overline{P}_{z,n};\frac{1}{2}\big)\,\Delta z$, $s_{z,C} = s_C - \frac{1}{r_C\Delta r}\left(\left(rF_r^{\text{hom}}\right)_e - \left(rF_r^{\text{hom}}\right)_w\right)$
4. Numerical complete flux
   - in r-direction: $\left(rF_r\right)_e = \left(rF_r^{\text{hom}}\right)_e + \left(rF_r^{\text{inh}}\right)_e$
   - in z-direction: $F_{z,n} = F_{z,n}^{\text{hom}} + F_{z,n}^{\text{inh}}$

Writing the discrete conservation law (5) in compass notation, we find

$$\Big(\left(rF_r\right)_e - \left(rF_r\right)_w\Big)\Delta z + r_C\big(F_{z,n} - F_{z,s}\big)\Delta r = r_C\,s_C\,\Delta r\,\Delta z. \tag{23}$$

Substitution of the numerical fluxes presented above leads to a 9-point stencil for the unknown φ. The complete flux scheme reduces to the homogeneous flux scheme if we set all coefficients $\gamma_{*,*}$ and $\delta_{*,*}$ to zero.

5 Numerical experiments

We study the following model problem to test the accuracy of the new complete flux (CF) scheme and to compare it with the homogeneous flux (HF) scheme. The problem domain is given by $1 \leq r \leq 4$, $0 \leq z \leq 3$. The unknown φ satisfies the partial differential equation $\nabla \cdot (\mathbf{u}\varphi - \varepsilon \nabla \varphi) = s$ in $(1,4) \times (0,3)$. We take $\mathbf{u}(r,z) = u_r \mathbf{e}_r + u_z \mathbf{e}_z = \frac{2}{r}\mathbf{e}_r + 3\mathbf{e}_z$. We impose Dirichlet boundary conditions and choose the source term s such that the analytical solution is given by $\varphi(r,z) = r^2 + 2r + 3z^2 + 4z + 5$. We discretize the PDE on a uniform grid (r_i, z_j) with N_r grid points in r-direction and N_z points in z-direction.

Numerical results are presented in Table 1. The error provided is the infinity-norm, so $e := \max_{i,j} \left| \varphi(r_i, z_j) - \varphi_{i,j} \right|$, with $\varphi_{i,j}$ the numerical approximation computed using the CF or HF scheme. The columns labelled 'quotient' list the quotient of the errors on successive grids. Both the HF and CF schemes show second order accuracy for dominant diffusion; HF reduces to first order for dominant advection. Note that the error of the CF scheme is a factor 2 smaller for dominant diffusion, and it is orders of magnitude more accurate for dominant advection.

Table 1 Numerical results for dominant diffusion ($\varepsilon = 10^{8}$) and dominant advection ($\varepsilon = 10^{-8}$).

	$\varepsilon = 10^{8}$				$\varepsilon = 10^{-8}$			
$N_r = N_z$	error HF	quotient	error CF	quotient	error HF	quotient	error CF	quotient
6	4.6862e-03		2.0625e-03		4.5491e+00		7.6891e-01	
11	1.2442e-03	3.766	6.0227e-04	3.425	2.5988e+00	1.750	2.0921e-01	3.675
21	3.1414e-04	3.961	1.5588e-04	3.864	1.3886e+00	1.872	5.4816e-02	3.817
41	7.9087e-05	3.972	3.9466e-05	3.950	7.2017e-01	1.928	1.4213e-02	3.857
81	1.9783e-05	3.998	9.8865e-06	3.992	3.6794e-01	1.957	3.6174e-03	3.929
161	4.9464e-06	3.999	2.4729e-06	3.998	1.8647e-01	1.973	9.1393e-04	3.958
321	1.2366e-06	4.000	6.1830e-07	3.999	9.4064e-02	1.982	2.2996e-04	3.974
641	3.0916e-07	4.000	1.5459e-07	4.000	4.7314e-02	1.988	5.7721e-05	3.984

References

1. Eymard, R., Gallouët, T., Herbin, R.: Finite volume methods. In: P.G. Ciarlet, J.L. Lions (eds.) Handbook of numerical analysis, vol. VII, pp. 713–1020. Elsevier, North-Holland (2000)
2. Liu, L.: Studies on the discretization of plasma transport equations. Ph.D. thesis, Eindhoven University of Technology, Eindhoven (2013)
3. ten Thije Boonkkamp, J.H.M., Anthonissen, M.J.H.: The finite volume-complete flux scheme for advection-diffusion-reaction equations. Journal of Scientific Computing **46**(1), 47–70 (2011)

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