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Very high-order finite volume scheme for 1D convection diffusion problem: 
the implicit case

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Abstract. We present a fourth-order in space, second-order in time finite volume scheme for transient convection diffusion problem based on the Polynomial Reconstruction Operator and a Crank-Nicholson method. A detailed description of the scheme is provided and we perform numerical tests to highlight the performance of the method in comparison with the classical Patankar method.

Keywords: Finite Volume; very high-order; transient convection-diffusion; Polynomial Reconstruction Operator (PRO).

1 Introduction

Efficient numerical schemes to solve convection diffusion equations is a constant challenge due to the wide range of problems which concern the coupling of the two major physical phenomena. Finite difference and finite element methods are very popular to produce numerical approximations ([1–3]) and a lot of academic and commercial codes are based on such techniques. The finite volume method for convection diffusion equations has been introduced in the sixties ([4, 5]) but did not receive attention during three decades whereas the finite element method has known a wide expansion. In the early eighties, the finite volume method reappeared with the original book of Patankar ([6]) for structured meshes and widely employed by engineers and physicists. Indeed, the method appears to be an interesting alternative due to its simplicity (one information per cell), the built-in conservative property, and the capacity to handle unstructured and non-conformal meshes. Important developments took place in this way and several classes of methods have been proposed. First, the original Patankar scheme for structured meshes has been extended to the non-structured case where an orthogonality condition is required to allow admissible diffusion flux (FV4 scheme [7–10]). The diamond scheme based on a local reconstruction of the gradient on each edge has been introduced by [11–13] while a finite volume scheme based on primal and dual meshes (DDFV scheme) has been proposed and developed by [14–16]. In the last six years, new techniques to design efficient finite volume schemes have been developed and a large proposal of numerical algorithms is now available such as the mixed-hybrid schemes ([17, 18]), mimetic schemes ([19, 20]), and schemes based on a local polynomial reconstruction ([21–23]).

Despite a constant effort to improve the schemes, a serious drawback of the finite volume method is the large amount of numerical viscosity and the weak convergence rate (at most second-order convergence). In the finite volume context, mean values are the fundamental data and the traditional (and implicit) identification "mean values = point-wise value at centroid" used by most of the authors is responsible of the discrepancy leading to, at most, a second-order scheme. The fact to reject such an identification is the crucial aspect of the presented method to provide fourth-order accuracy schemes. The main tool of the method is a local polynomial reconstruction in which the coefficients are determined from the mean values of the neighboring cells ([24, 25]). Another important issue is the choice of the reconstruction in function of the differential operator type. For the convective operator, we only employ internal values, i.e. mean-values on the cells, to determine the reconstructed polynomial function, whereas we introduce the Dirichlet conditions in the polynomial reconstruction employed in the diffusive operator to enforce
the boundary conditions.

This paper is devoted to a new class of finite volume schemes for transient convection-diffusion problem able to reach a fourth-order in space and second-order in time. We present the method for the one-dimensional case to detail the scheme with simple examples considering the convection-diffusion equation with the formulation

\[
\begin{align*}
\partial_t u - \partial_x (a \partial_x u) + \partial_x (v u) &= f & \text{on } & \Omega \times ]0, T[ \\
u(0, t) &= u_0(t), & u(1, t) &= u_{tg}(t), & u(x, 0) &= u^0(x),
\end{align*}
\]

where \( \Omega : = ]0, 1[ \), \( a \) (the diffusive coefficient) and \( v \) (the convective coefficient) are regular functions on \( \Omega \times ]0, T[ \) with \( a(x, t) \geq \alpha > 0 \), while \( f = f(x, t) \) represents a regular source term.

The rest of the paper is as follows. The second section recalls the classical finite volume scheme for convection-diffusion problem (namely the Patankar method). Then, we introduce several polynomial reconstructions in section three, while the fourth section is devoted to the high-order finite volume schemes. The next section concerns the numerical tests to show the scheme capacity to provide fourth-order in space and second-order in time accuracy both for the convective and the diffusive part of the operator. In the last section we present the conclusions and extensions.

## 2 Patankar finite volume schemes

To design the numerical schemes, we denote by \( \mathcal{T}_h \) a mesh of \( \Omega \) constituted of cells \( K_i : = [x_{i-1/2}, x_{i+1/2}], i = 1, \ldots, I \), with centroid \( c_i \), where \( x_{1/2} := 0 \) and \( x_{i+1/2} := x_{i-1/2} + h_i \), and set \( h_i \) as the ratio between the length of two consecutive cells, that is \( h_i := h_i/h_{i+1}, i = 1, 3, \ldots, I - 1 \) (cf. Fig. 1). In the same way, we consider a subdivision \( (t^n)_{n=0, \ldots, N} \) of the time interval \([0, T]\) with \( t^{n+1} := t^n + \delta^{n+1/2} \).

In the finite volume context, \( u_i \) denotes an approximation of the mean value over cell \( K_i \), that is

\[
u^n_i \approx \frac{1}{h_i} \int_{K_i} u(x, t^n) \, dx,
\]

and vector \( U^n = (u^n_0, \ldots, u^n_I)^T \in \mathbb{R}^I \) is the vector of the unknowns at time \( t^n \).

For the sake of consistency, we recall the Patankar scheme. For each interface \( x_{i+1/2}, i = 0, \ldots, I \), we define the diffusive and the convective fluxes for any vector \( U \in \mathbb{R}^I \) by

\[
\mathcal{F}_{\text{diff},i+\frac{1}{2}}^P(U) := a(x_{i+\frac{1}{2}}) \frac{2(u_{i+1} - u_i)}{(h_i + h_{i+1})}
\]

and

\[
\mathcal{F}_{\text{conv},i+\frac{1}{2}}^P(U) := [v(x_{i+\frac{1}{2}})]^+ u_i + [v(x_{i+\frac{1}{2}})]^- u_{i+1},
\]

respectively, where we have set \( h_0 := 0, h_{I+1} := 0, u_0 = u_{tg}, u_{I+1} = u_{tg} \) and we used the notation \([\alpha]^+ := (\alpha + |\alpha|)/2, [\alpha]^- := (\alpha - |\alpha|)/2\). Note that we have skip the time index for the sake of simplicity. Then we defined the finite volume operator for cell \( K_i \) associated to the Patankar fluxes (1)-(2) by

\[
\mathcal{G}_i^P(U; u_{tg}, u_{tg}, f) := - \left[ \mathcal{F}_{\text{diff},i+\frac{1}{2}}^P(U) - \mathcal{F}_{\text{diff},i-\frac{1}{2}}^P(U) \right] + \left[ \mathcal{F}_{\text{conv},i+\frac{1}{2}}^P(U) - \mathcal{F}_{\text{conv},i-\frac{1}{2}}^P(U) \right] - h_i f_i.
\]
where \( f_i \) is an approximation of the mean value of \( f \) over cell \( K_i \), that is
\[
f_i \approx \frac{1}{h_i} \int_{K_i} f \, dx.
\]

Using expression (3), we define the semi-discrete problem: find \( U(t) = (u_1(t), \ldots, u_I(t))^T \) such that
\[
\frac{dU}{dt} + \mathcal{G}^P(U; u_{if}, u_{rg}, f) = (0, \ldots, 0)^T
\]
\[
U(0) = U^0, \quad u_0(t) = u_{if}(t), \quad u_{I+1}(t) = u_{rg}(t),
\]
with
\[
U^0 := (u_1^0, \ldots, u_I^0)^T, \quad u_i^0 := \frac{1}{h_i} \int_{K_i} u_i^0 \, dx, \quad i = 1, \ldots, I,
\]
and
\[
\mathcal{G}^P(U; u_{if}, u_{rg}, f) := (\mathcal{G}_1^P(U; u_{if}, u_{rg}, f), \ldots, \mathcal{G}_I^P(U; u_{if}, u_{rg}, f))^T \in \mathbb{R}^I
\]
being the finite volume operator for the mesh \( T_h \).

The three classical time discretizations are

- the explicit scheme:
  \[
  \mathcal{H}^P(U^{n+1}; U^n, u_{if}, u_{rg}, f) := \frac{U^{n+1} - U^n}{\delta n+1} + \mathcal{G}^P(U^n; u_{if}, u_{rg}, f);
  \]

- the implicit scheme:
  \[
  \mathcal{H}^P(U^{n+1}; U^n, u_{if}, u_{rg}, f) := \frac{U^{n+1} - U^n}{\delta n+1} + \mathcal{G}^P(U^n; u_{if}, u_{rg}, f);
  \]

- the Crank-Nicholson scheme:
  \[
  \mathcal{H}^P(U^{n+1}; U^n, u_{if}, u_{rg}, f) := \frac{U^{n+1} - U^n}{\delta n+1/2} + \frac{1}{2} \mathcal{G}^P(U^n; u_{if}, u_{rg}, f) + \frac{1}{2} \mathcal{G}^P(U^{n+1}; u_{if}, u_{rg}, f).
  \]

In each case, one has to determine the vector \( U^{n+1} \) solution of the affine problem
\[
\mathcal{H}^P(U; U^n, u_{if}, u_{rg}, f) = 0, \quad U \in \mathbb{R}^I.
\]

3 The polynomial reconstructions

The main tool to provide very high-order approximations is the construction of a specific polynomial approximation. In the sequel, we shall consider two kinds of reconstructions. For each cell \( K_i, i = 1, \ldots, I \), we denote by \( \nu(i) \) the stencil associated to it such that \( i \notin \nu(i) \), i.e. a set of neighboring cells, and by \( u_i(x; \nu(i), d) \in \mathbb{P}_d \) the polynomial reconstruction on cell \( K_i \) of degree \( d \) based on the stencil \( \nu(i) \).

In practice, we build the stencil \( \nu(i) \) in function of the polynomial degree \( d \) we shall reconstruct picking up the nearest \( d + 1 \) cells to \( K_i \). A difficulty arises when dealing with cells which share a point with the boundary. The two proposed reconstructions vary in the manner that the boundary conditions are considered.

3.1 Design of polynomial \( \hat{u}_i(x; \nu(i), d) \)

For each cell \( K_i, i = 1, \ldots, I \), we consider the polynomial expression (we skip the \( \nu(i) \) reference for the sake of simplicity)
\[
\hat{u}_i(x; d) := u_i + \sum_{\alpha=1}^{d} \hat{R}_{\alpha} \left( \frac{(x - c_{i})^\alpha}{\delta h} - \frac{1}{h_i} \int_{K_i} (x - c_{i})^\alpha \, dx \right),
\]
where the coefficients \( \hat{R}_{\alpha}, \alpha = 1, \ldots, d \), are the minimizers of the functional
\[
\hat{E} \left( \hat{R}_{\alpha} \right) := \sum_{j \in \nu(i)} \left[ \frac{1}{h_j} \int_{K_j} \hat{u}_i(x; d) \, dx - u_j \right]^2, \quad i = 1, \ldots, I.
\]
To provide the numerical flux at the boundary for the convective flux, we use the extension \( \hat{u}_0 := u_{if} \) and \( \hat{u}_{I+1} := u_{rg} \) and we denote by \( \hat{P}(U; d) = (\hat{u}_0(x; d), \ldots, \hat{u}_{I+1}(x; d))^T \) the vectorial function on \( \Omega \) associated to the \( \hat{u} \) polynomial reconstruction.
4.2 The semi-discrete formulation

The semi-discrete problem consists in solving the affine system of \( I \) differential equations with the initial condition \( U(0) = (u_{1}^{0}, \ldots, u_{I}^{0})^{T} \).
4.3 Time discretization
As in the Patankar case, we introduce the three classical time discretizations, namely

- the explicit scheme:
  \[ \mathcal{H}^{\text{PRO}}(U^{n+1}; U^n, \delta^{n+1/2}, u_{\text{lf}}, u_{\text{rg}}, f, d) := \frac{U^{n+1} - U^n}{\delta^{n+1/2}} + G^{\text{PRO}}(U^n; u_{\text{lf}}, u_{\text{rg}}, f, d); \]

- the implicit scheme:
  \[ \mathcal{H}^{\text{PRO}}(U^{n+1}; U^n, \delta^{n+1/2}, u_{\text{lf}}, u_{\text{rg}}, f, d) := \frac{U^{n+1} - U^n}{\delta^{n+1/2}} + G^{\text{PRO}}(U^n+1; u_{\text{lf}}, u_{\text{rg}}, f, d); \]

- the Crank-Nicholson scheme:
  \[ \mathcal{H}^{\text{PRO}}(U^{n+1}; U^n, \delta^{n+1/2}, u_{\text{lf}}, u_{\text{rg}}, f, d) := \frac{U^{n+1} - U^n}{\delta^{n+1/2}} + \frac{1}{2} G^{\text{PRO}}(U^n; u_{\text{lf}}, u_{\text{rg}}, f, d) + \frac{1}{2} G^{\text{PRO}}(U^{n+1}; u_{\text{lf}}, u_{\text{rg}}, f, d). \]

In each case, one has to determine the vector \( U^{n+1} \) solution of the affine problem
\[ \mathcal{H}^{\text{PRO}}(U; U^n, \delta^{n+1/2}, u_{\text{lf}}, u_{\text{rg}}, f, d) = (0, \ldots, 0)^T, \quad U \in \mathbb{R}^I. \]

5 Numerical tests
Numerical simulations have been carried out to check the convergence order of the methods and show its effectiveness. Two kinds of convergence has to be investigated: one with respect to space discretization and the other with respect to time discretization.

In the following subsections, the error between the solution and its approximation is provided with \( L^\infty \) norm since we deal with regular functions, namely
\[ E_0 := \max_{i=1}^I |u_i^N - \bar{u}_i^N|, \]
where
\[ \bar{U} := (\bar{u}_1^N, \ldots, \bar{u}_I^N), \quad \bar{u}_i^N := \frac{1}{h_i} \int_{K_i} u(x, T) \, dx, \]
are the exact mean values of the solution of the continuous problem at time \( t = T \). Note that \( E_0 \) does not depend on the polynomial reconstruction but just on the mean values.

For the sake of simplicity, we consider a uniform discretization in space and time controlled by parameters \( h \) and \( \Delta t \) so we set \( h := h_i = \frac{1}{I}, \quad t = 1, \ldots, I, \) and \( \delta^{n+1/2} := \Delta t, \quad n = 0, \ldots, N. \)

We will present two examples. In both of them, we have as the analytical solution \( a(x, t) = \sin(2\pi x) \exp(-t) \). We take \( a(x) = 1 \) and \( v = 0 \) to provide a pure diffusion problem in the first example, while we consider a convection diffusion problem with \( a(x) = 1 \) and \( v = 1 \) in the second one. All the computations are performed using the Crank-Nicholson scheme in time till we reach the final time \( T = 0.1 \).

5.1 Example 1
As mentioned above, we first start with the transient diffusion equation. To measure the convergence rate deriving from the Crank-Nicholson method, we fix the number of cells large enough to guaranty a smaller error for the space approximation than the error deriving from the scheme in time. As expected, Table 1 shows that we get a second-order convergence both for the Patankar and the PRO-P2 scheme (see the convergence curve in Figure 2). Note that we need 3200 cells to eliminate the error in space for Patankar while we only use 120 cell with the PRO-scheme. Another point is the better condition number of the linear system when using the PRO-scheme.
Table 1: Example 1 — convergence in time.

<table>
<thead>
<tr>
<th>$\Delta t$</th>
<th>$k(A)$</th>
<th>$E_0$ err ord</th>
<th>$k(A)$</th>
<th>$E_0$ err ord</th>
</tr>
</thead>
<tbody>
<tr>
<td>1/10</td>
<td>1.4E+06 1.6E−03 NA</td>
<td>1.7E+03 1.6E−03 NA</td>
<td></td>
<td></td>
</tr>
<tr>
<td>1/20</td>
<td>8.2E+05 2.9E−04 2.5</td>
<td>1.0E+03 2.9E−04 2.5</td>
<td></td>
<td></td>
</tr>
<tr>
<td>1/40</td>
<td>4.6E+05 7.1E−05 2.0</td>
<td>5.7E+02 7.0E−05 2.1</td>
<td></td>
<td></td>
</tr>
<tr>
<td>1/80</td>
<td>2.4E+05 1.7E−05 2.0</td>
<td>3.0E+02 1.7E−05 2.1</td>
<td></td>
<td></td>
</tr>
<tr>
<td>1/160</td>
<td>1.2E+05 4.1E−06 2.0</td>
<td>1.6E+02 3.7E−06 2.2</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Figure 2: Example 1 — convergence curves of $E_0$ in time for a fixed value of $I$: $I = 3200$ for the Patankar scheme and $I = 120$ for the PRO-FV scheme $P_3$ (cf. Table 1).

We now check the convergence rate in space. To this end, we fix the time step small enough to ensure a neglected error in time. We obtain a predominant mass matrix leading to a small conditioning number but we need large number of iterations to reach the final time $T$. As shown in Table 2, we obtain a second-order scheme with the Patankar method, whereas an accurate and effective fourth-order is achieved with the PRO-$P_3$ scheme. For 160 cells the error is cut by around 1000 with a smaller computational effort (see Figure 3 for the convergence curves).

Table 2: Example 1 — convergence in space with fixed $\Delta t = 1/1600$.

<table>
<thead>
<tr>
<th>$I$</th>
<th>$k(A)$</th>
<th>$E_0$ err ord</th>
</tr>
</thead>
<tbody>
<tr>
<td>20</td>
<td>1.5E+00</td>
<td>7.4E−03 NA</td>
</tr>
<tr>
<td>40</td>
<td>3.0E+00</td>
<td>1.9E−03 2.0</td>
</tr>
<tr>
<td>80</td>
<td>9.0E+00</td>
<td>4.7E−04 2.0</td>
</tr>
<tr>
<td>160</td>
<td>3.3E+01</td>
<td>1.2E−04 2.0</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>$I$</th>
<th>$k(A)$</th>
<th>$E_0$ err ord</th>
</tr>
</thead>
<tbody>
<tr>
<td>20</td>
<td>1.4E+00</td>
<td>1.8E−03 NA</td>
</tr>
<tr>
<td>40</td>
<td>2.7E+00</td>
<td>7.2E−05 4.7</td>
</tr>
<tr>
<td>80</td>
<td>8.0E+00</td>
<td>3.7E−06 4.3</td>
</tr>
<tr>
<td>160</td>
<td>2.9E+01</td>
<td>1.7E−07 4.4</td>
</tr>
</tbody>
</table>
Since the schemes in time and space have not the same order, it is numerically important to adapt the time step with the space step. For the Patankar scheme with Crank-Nicholson method, we have both a second-order scheme so we set $\Delta t = h$. Since the PRO-$P_3$ provides a fourth-order in space, we set $\Delta t = h^2$ and expect a fourth-order convergence. Table 3 confirms the good choice of the time step and we get a global second-order scheme with Patankar and a global fourth-order scheme with the PRO method.

### Table 3: Example 1 — convergence in space.

<table>
<thead>
<tr>
<th>$I$</th>
<th>$k(A)$</th>
<th>$E_0$</th>
<th>ord</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>err</td>
<td></td>
</tr>
<tr>
<td>10</td>
<td>1.4E+01</td>
<td>4.0E-02</td>
<td>NA</td>
</tr>
<tr>
<td>20</td>
<td>3.3E+01</td>
<td>7.3E-03</td>
<td>2.5</td>
</tr>
<tr>
<td>Patankar ($\Delta t = h$)</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>40</td>
<td>7.2E+01</td>
<td>1.8E-03</td>
<td>2.0</td>
</tr>
<tr>
<td>80</td>
<td>1.5E+02</td>
<td>4.5E-04</td>
<td>2.0</td>
</tr>
<tr>
<td>160</td>
<td>3.1E+02</td>
<td>1.1E-04</td>
<td>2.0</td>
</tr>
<tr>
<td>$P_3$ ($\Delta t = h^2$)</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>10</td>
<td>2.6E+00</td>
<td>3.9E-02</td>
<td>NA</td>
</tr>
<tr>
<td>20</td>
<td>2.7E+00</td>
<td>1.8E-03</td>
<td>4.4</td>
</tr>
<tr>
<td>40</td>
<td>2.7E+00</td>
<td>7.2E-05</td>
<td>4.7</td>
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<tr>
<td>80</td>
<td>2.7E+00</td>
<td>3.7E-06</td>
<td>4.3</td>
</tr>
<tr>
<td>160</td>
<td>2.7E+00</td>
<td>2.1E-07</td>
<td>4.1</td>
</tr>
</tbody>
</table>

### 5.2 Example 2

The second example deals with the transient convection diffusion problem with $a(x) = 1$ and $v = 1$, and we choose the right-hand side term such that $u(x) = \sin(2\pi x) \exp(-t)$ is the solution. Based on the previous numerical experiences, we use $\Delta t = h$ for the Patankar-Crank-Nicholson scheme and $\Delta t = h^2$ for the PRO-Crank-Nicholson scheme. We print out in Table 4 the global convergence rate and obtain a first-order rate of convergence for the classical method due to the rough discretization of the convective part (just an upwind method). We obtain an effective fourth-order convergence with the PRO scheme which highlights the effectiveness of the method.
Table 4: Example 2 \((u(x) = \sin(2\pi x) \exp(-t), a(x) = 1, v = 1)\) with Crank-Nicholson

<table>
<thead>
<tr>
<th>(I)</th>
<th>(k(A))</th>
<th>(E_{\text{err}})</th>
<th>(\text{ord} )</th>
</tr>
</thead>
<tbody>
<tr>
<td>10</td>
<td>1.4E+01</td>
<td>2.1E−02</td>
<td>NA</td>
</tr>
<tr>
<td>20</td>
<td>3.3E+01</td>
<td>1.5E−02</td>
<td>0.5</td>
</tr>
<tr>
<td>Patankar ((\Delta t = h))</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>40</td>
<td>7.3E+01</td>
<td>9.9E−03</td>
<td>0.6</td>
</tr>
<tr>
<td>80</td>
<td>1.5E+02</td>
<td>5.5E−03</td>
<td>0.9</td>
</tr>
<tr>
<td>160</td>
<td>3.1E+02</td>
<td>2.9E−03</td>
<td>0.9</td>
</tr>
<tr>
<td>(P_3) ((\Delta t = h^2))</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>10</td>
<td>2.7E+00</td>
<td>3.3E−02</td>
<td>NA</td>
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<td>1.7E−03</td>
<td>4.2</td>
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<td>4.2</td>
</tr>
<tr>
<td>160</td>
<td>2.8E+00</td>
<td>2.3E−07</td>
<td>4.1</td>
</tr>
</tbody>
</table>

6 Conclusion

We have presented a new finite volume method for one-dimensional convection-diffusion problem which provides very high-order accuracy. Numerical simulations have been carried out to prove the capacity of the method to effectively reach the fourth-order accuracy. Several extensions are under consideration. The two- and three-dimensional case is of course of crucial importance, but we will also investigate the schemes for both Dirichlet and Neumann boundary conditions. Another difficulty concerns the solution stability when dealing with rough data. A strategy based on the MOOD method ([24, 25]) is currently being developed.

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7 Bibliography

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