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Numerical approximation of parabolic problems by residual distribution schemes

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SUMMARY

We are interested in the numerical approximation of steady scalar convection–diffusion problems by means of high order schemes called Residual Distribution schemes. In the inviscid case, one can develop nonlinear Residual Distribution schemes that are nonoscillatory, even in the case of very strong discontinuities, while having the most possible compact stencil, on hybrid unstructured meshes. This paper proposes and compare extensions of these schemes for the convection–diffusion problem. This methodology, in particular in terms of accuracy, is evaluated on problem with exact solutions. Its nonoscillatory behavior is tested against the Smith and Hutton problem. Copyright © 2012 John Wiley & Sons, Ltd.

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1. INTRODUCTION

We are interested in the approximation of convection–diffusion problems such as

$$\begin{array}{rll} \text{div } f(u) = \text{div } (\mathbf{D}\nabla u), & & x \in \Omega \\ u = g_S & \text{on } \Gamma_S \subset \partial\Omega & \\ u = g_W & \text{on } \Gamma_W \subset \partial\Omega & \end{array} \tag{1}$$

where the function f is C^1 function and $\mathbf{D}$ is a $d \times d$ matrix, which symmetric part $(\mathbf{D} + \mathbf{D}^T)/2$ is positive definite. The functions g_S and g_W used in the Dirichlet and Neuman conditions are assumed regular enough so that the problem is well-posed.‡ In (1), $\partial\Omega$ is the boundary of $\Omega \subset \mathbb{R}^d$, $\Gamma_s \cup \Gamma_w = \Omega$. The ultimate goal is the approximation of the Navier–Stokes equations, but this is out of the scope of this paper: we focus only on the scalar case.

The numerical setting is the following. The domain Ω is discretized by means of an unstructured grid $\mathcal{T}_h$, and to fix ideas, we assume that $\Omega \subset \mathbb{R}^2$ and that the elements of the mesh $\mathcal{T}_h$ are triangles. None of these two assumptions is essential by any mean. In the setting of this paper, we seek for an approximation to the values of the solution of (1) at the vertices of the mesh and at additional points that correspond to the equispaced interpolation points associated to the standard Lagrange approximation. For example, in the third-order case, in addition to the vertices, we also consider the midpoints of the edges; in the fourth-order case, we consider vertices, plus (in 2D) cell centers and two additional equispaced edge points, and so forth. Note that other type of degrees of freedom

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‡That is, the measure of Γ_D is strictly positive, and the Dirichlet and Newman conditions are in $H^{1/2}(\Gamma_S)$ (respectively $H^{1/2}(\Gamma_W)$).

can be considered (see e.g., [1]). The key point here is that one is able to reconstruct a continuous interpolant u^h from the degrees of freedom. Here, $u^h \in V^h$, where

$$V^h = \left\{ u \in H^1(\Omega), u_{|K} \in \mathbb{P}^k(K) \text{ for any element } K \right\}.$$

We focus on C^0 continuous approximations and on the steady problem (1). However, our discussion can be generalized to discontinuous approximations, see [2,3], and to unsteady problems, see [4–6].

We are interested in the approximation of (1) using Residual Distribution (RD) schemes. If one denotes by $\{\sigma_\ell\}_{\ell=1,\ldots,n_{\text{dof}}}$ the set of degrees of freedom, a RD scheme writes as follows: for any σ_ℓ, find $u^h \in V^h$ such that

$$\sum_{K,\sigma_\ell \in K} \phi^K_{\sigma_\ell}(u^h) = 0. \tag{2a}$$

The residuals $\phi^K_{\sigma_\ell}(u^h)$ in the case $\mathbf{D} \equiv 0$ satisfy the following conservation relation:

$$\sum_{\sigma \in K} \phi^K_{\sigma}(u^h) = \int_{\partial K} f^h(u^h) \cdot \vec{n} \mathrm{d}\partial K \tag{2b}$$

where $f^h(u^h)$ is a convergent interpolant of $f(u)$ (e.g., $f(u^h)$ or the Lagrange interpolant of $f(u)$). One of the key requirement is that the flux approximation $f^h(u^h) \cdot \vec{n}$ is continuous across the edges of K, whatever the element K is.

The approximation of the nondiffusive problem $\mathbf{D} \equiv 0$ (with slightly modified boundary conditions) is now a standard matter, even for high order of accuracy. In the inviscid case, the schemes are formally high-order accurate, and the focus is on the L^∞ stability of the scheme. The objective of the paper is to propose extensions of these approximations to the viscous problem (1), in particular correct generalizations of the relations (2). We wish to keep the accuracy property without sacrificing the convergence towards weak solutions and the L^∞ stability, that is, the shock capturing capability of the numerical scheme, especially when the diffusion matrix tends to 0.

The numerical approximation of (1) has already been considered by several authors. It is not, however, a completely trivial matter, and we believe there is still work to do. Indeed, the class of RD schemes has originally been devised for (steady) transport problems, on the basis of a genuinely multidimensional upwind approach. Among the very first contributions, one may quote the work of P. L. Roe [7] and R.-H. Ni [8]. Some connections with more classical schemes, such as the streamline diffusion method by Hughes, Johnson, and co-authors, have soon been made [9]. However, the main problem is that, even though some RD schemes can be recast as a particular class stabilized finite elements with emphasis on L^∞ stability, there is no clear general framework allowing to choose the test functions to recover a traditional variational statement. The main reason of this problem is related to the underlying formulation: everything is seen from a discrete point of view, and emphasis is put on the pointwise behavior of the residual. There is no surprise here since the focus is on the L^∞ stability. Indeed, the same remark applies to variants of the method not aiming at approximating point values of the solution, as in [1]. In this case, the local discrete pointwise residuals are replaced by residuals for polynomial coefficient sets for which once again a maximum principle is sought for.

There has been already many works on the approximation of (1) by means of RD. In addition to early works where the RD scheme for the nonviscous (1) was coupled, for $\mathbb{P}^1$ elements, to the Galerkin approximation of the viscous terms, one may quote the work of Caraeni [10], and more recently that of Villedieu *et al.* [11,12] where this path has been explored further for scalar problems and for the Navier–Stokes equations. A different approach is being pursued by Nishikawa [13–15], for second order of accuracy, on the basis of a re-interpretation of the solution of (1) as the steady solution of a hyperbolic relaxation system. The difference between our approach and [10] is that our technique is probably simpler, and the memory footprint is probably less important. Caraeni's method relies on the use of a gradient reconstruction that has the flavor of what is carried out in high-order finite volume methods and thus has a much wider stencil, especially when higher accuracy is sought for. We believe our method to be more systematic. The difference between [11, 12] is that

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our method is able to handle very large gradients. In [13–15], only second-order accuracy is sought for; nevertheless, this contribution has been a source of inspiration for the present work.

In this paper, we are interested in gaining a better understanding of the ideas discussed in the aforementioned references to be able to handle (1) in a more general setting. In particular, we are interested in a formal accuracy higher than second, and to discretizations that are L^∞ stable, at least in the limit $\mathbf{D} \to 0$. The key point of the analysis is a variational formulation of the inviscid RD scheme that is then formally extended to the viscous case in the spirit of what is carried out for the Discontinuous Galerkin schemes, although keeping the same degrees of freedom as for the inviscid case.

The presentation is organized as follows. We first recall a remark of [16] in the $\mathbb{P}^1$ case (second order of accuracy). This remark allows to explain why a simple coupling between the L^∞ stable RD scheme and a simple Galerkin approximation of the viscous term is still a residual method. Then, we show, by a counter example, that this remark cannot be generalized: it only works on $\mathbb{P}^1$ elements. To overcome this drawback, we revisit the formulation of the nonviscous scheme and propose a nonstandard variational formulation of these schemes that enables a generalization of the relations (4), in particular the conservation relation (4a), and thus a formulation of the scheme in the viscous case. Numerical tests are performed to check the numerical accuracy, in particular with respect to variations of the values of the viscosity. We also investigate the nonoscillatory properties of the method.

2. SOME BASIC INFORMATION ABOUT RESIDUAL DISTRIBUTION SCHEMES IN THE CASE $\mathbf{D} \equiv 0$

The problem is to find an approximate solution of

$$\operatorname{div} f(u) = 0, \qquad x \in \Omega \tag{3a}$$

where the boundary conditions, when $D = 0$, are

$$u = g \text{ on } \Gamma_- = \{M \in \partial\Omega, \nabla_u f(u) \cdot \vec{n} < 0\}, \tag{3b}$$

and $\vec{n}$ is the inward normal to $\partial\Omega$ at $M \in \Omega$.

Let us denote by $\mathcal{S}$ the set of degrees of freedom σ that are needed to represent

$$V_h = \{v \in L^2(\Omega), \text{ for any } K \in \mathcal{T}_h, v_{|K} \in \mathbb{P}^r(K)\} \cap \{v \in L^2(\Omega), v_{|\Gamma_-} = g\}$$

the set of functions where we are looking for a solution. There is some abuse of notations in this "definition". Since the elements of $v \in V_h$ are polynomials of degree r in any triangle of $\mathcal{T}_h$, the degrees of freedom are, in this paper, the solution values at Lagrange points: the vertices for $\mathbb{P}^1$, the vertices and the edge midpoints for $\mathbb{P}^2$, and so forth.

Given any $u^h \in V^h$, we define two types of residuals as follows:

1. For any $K \in \mathcal{T}_h$ and any σ degree of freedom in K, the element residuals $\phi_\sigma^K(u^h)$ must sum up to the total residual $\phi^K(u^h)$,

$$\sum_{\sigma \in K} \phi_\sigma^K(u^h) = \phi^K(u^h) := \int_{\partial K} f^h(u^h) \cdot \vec{n} \, \mathrm{d}\partial K. \tag{4a}$$

2. For any boundary edge $\Gamma \subset \Gamma_-$ and any σ degree of freedom in Γ, the edge residuals $\phi_\sigma^\Gamma(u^h)$ must sum up to the total edge residual $\phi^\Gamma(u^h)$,

$$\sum_{\sigma \in \Gamma} \phi_\sigma^\Gamma(u^h) = \phi^\Gamma(u^h) := \int_\Gamma \left[f^h(u^h) \cdot \vec{n} - \hat{f}(u^h, g, \vec{n}) \right] \mathrm{d}\partial K. \tag{4b}$$

In (4b), $\hat{f}$ is a consistent numerical flux.

The two types of residuals must be continuous with respect to their arguments. The conditions (4), in addition to the continuity requirement of $f^h(u^h)$ across the edges of the triangulation and the

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consistency of the numerical flux $\hat{f}$, enable to prove a Lax–Wendroff (LW) theorem, see [17]. In practice, the total residuals and total edge residuals are evaluated by numerical quadratures.

The system (3) is approximated by the following: find $u^h \in V^h$ such that for any $\sigma \in \mathcal{T}^h$,

$$\begin{aligned} \sum_{K,\sigma\in K} \phi_\sigma^K &= 0 \qquad \text{for the internal degrees of freedom} \\ \sum_{K,\sigma\in K} \phi_\sigma^K + \sum_{\Gamma,\sigma\in\Gamma} \phi_\sigma^\Gamma &= 0 \qquad \text{if } \sigma \in \partial\Omega. \end{aligned} \tag{5}$$

In general, this leads to very nonlinear systems that are solved by an iterative technique. In this paper, we have used only a Jacobi-like iterative technique (i.e., simple forward Euler time stepping), although more sophisticated and more efficient methods can be used and are used for large scale problems.

The next question is how to define in practice the subresiduals. The first requirement is about accuracy. In [17], it is shown that if

$$\phi_\sigma^\Sigma = O(h^{d_\Sigma + r}),$$

for any mesh entity Σ (element or edge), d_Σ denoting its dimension[§], then the scheme is $r+1$ accurate, provided of course as usual that the mesh is regular in the finite element sense. We recall later in the text how this can be achieved in practice.

The second question is about stability. To do that, the standard technique is to compare the sign of the residuals with that of a monotone scheme. Following a path initiated by Roe and Abgrall[17], we show how it is possible to obtain *simultaneously* monotonicity preservation and accuracy. Unfortunately, in general, the technique proposed in [17] combined with an iterative scheme does not converge to a steady state. The main reason is that the nonlinear mechanism at the basis of the construction only involves the preservation of the signs of the discretization coefficients to guarantee a discrete maximum principle and a priori; no physical principle is involved in the procedure. In general, this leads to the appearance of mild spurious modes. A typical footprint of this behavior is a staircase appearance of the numerical solution. These difficulties are analyzed and solved in [18] for $\mathbb{P}^1$ elements and in [19, 20] for higher degree polynomials. The interested reader can consult these references for details. The key element is to modify the residuals $\phi_i^K(u^h)$ obtained following the approach of [17] as follows

$$\phi_i^{K\star}(u^h) = \phi_i^K(u^h) + \overbrace{\frac{h_K}{N_K} \sum_{x_q\in K} \Big(\nabla_u f(u^h)(x_q)\cdot\nabla\varphi_i\Big)\, \tau\, \Big(\nabla_u f(u^h)(x_q)\cdot\nabla u^h(x_q)\Big)}^{\mathcal{F}}, \tag{6}$$

with $N_K = \#\{\sigma, \sigma \in K\}$. The *filter* $\mathcal{F}$ in (6) has the flavor of

$$h_K \int_K \Big(\nabla_u f(u^h)\nabla\varphi_i\Big)\, \tau\, \Big(\nabla_u f(u^h)\cdot\nabla u^h\Big)\, \mathrm{d}K$$

evaluated via numerical quadrature. In [19], an analysis is conducted to understand what are the relations between the last integral and the filter $\mathcal{F}$. It is shown that the quadrature does not need to be consistent, but, since the role of this term is to act as a dissipation that vanishes on exact solutions, the paper gives a criterion to choose the points x_q for triangular/tetrahedrons and quadrangle/hexahedrons elements. In the linear case, the centroid of the cell K is fine for triangular elements, whereas in the quadratic (triangle) case, the triangle vertices are fine. Other kind of elements are analyzed in that reference. The parameter τ (a matrix in the system case) is also discussed, but the quality of solution has no real dependency on τ in practice: its role is mainly to satisfy some dimensional consistency principle.

The modification in (6) looks very much with the stabilization term in the Streamline Upwind Petrov Galerkin scheme, which itself has a lot to do with the artificial dissipation of the LW scheme.

[§]In 2D, $d_\Sigma = 1$ for an edge Γ and $d_\Sigma = 2$ for an element K.

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However, its role is *very* different: without this term, the scheme is perfectly stable in the L^∞ norm, but if one implements an iterative method to solve the system (5), the method will not converge. The role of $\mathcal{F}$ is to enable the iterative convergence, and hence to guaranty the accuracy. It is an experimental fact that the non oscillatory properties of the original scheme are not degraded in practice.

3. APPROXIMATION OF (1) IN THE $\mathbb{P}^1$ WITH TRIANGLE ELEMENTS CASE

In the $\mathbb{P}^1$ case, the degrees of freedom are simply the vertices of the mesh. To make things simpler, we assume $\mathbf{D} = \varepsilon\,\mathrm{Id}$. In the case, $\varepsilon = 0$, the RD scheme (2a) for (1) would write: for any mesh point i,

$$\sum_{K, i\in K} \phi_i^K(u^h) = 0 \tag{7}$$

where the residuals satisfy the conservation condition (2b)

$$\sum_{i\in K} \phi_i^K(u^h) = \phi^K := \int_{\partial K} f^h(u^h)\cdot\vec{n}\,\mathrm{d}\partial K. \tag{8}$$

In the following, we shall assume that the flux is linear, that is, $f(u) = \vec{\lambda}u$. The analysis can be generalized to nonlinear flux provided that $f^h(u^h)$ is the Lagrange interpolant of $f(u)$; this is what we do in practice. In the second-order case, the residual have the form

$$\phi_i^K = \beta_i^K \phi^K \tag{9}$$

where $\{\beta_i^K\}$ is uniformly bounded and constructed by various means, see Section 4.

Using the standard $\mathbb{P}^1$ shape function φ_i, we can rewrite ϕ^K in a Petrov Galerkin manner,

$$\phi_i^K = \int_K \varphi_i \nabla\cdot f^h(u^h)\mathrm{d}K + \int_K \left(\beta_i^K - \frac{1}{3}\right)\nabla\cdot f^h(u^h)\mathrm{d}K := \int_K \omega_i^K \nabla\cdot f^h(u^h)\mathrm{d}K$$

because $f^h(u^h)$ is a linear polynomial so that $\nabla\cdot f^h(u^h)$ is a constant and $\int_K \varphi_i\,dK = |K|/3$ in the case of a triangle. In this formulation, ω_i is not continuous across edges and then cannot be used to approximate (1).

In [16], it was noticed that the *same* scheme could be written differently. Denote b_K the hat function that is 0 on ∂K and 1 at the gravity center of K. It is a piecewise linear function that satisfies

$$\int_{\partial K} \nabla b^K\cdot\vec{n}\,\mathrm{d}\partial K = 0 \text{ and } \int_K b^K \mathrm{d}K > 0.$$

We can write

$$\phi_i^K = \beta_i^K\phi^K = \int_K \varphi_i\nabla\cdot f^h(u^h)\mathrm{d}K + \gamma_i^K\int_K b^K\nabla\cdot f^h(u^h)\mathrm{d}K$$

with

$$\gamma_i^K\int_K b^K\mathrm{d}K = \left(\beta_i^K - \frac{1}{3}\right)|K|$$

again because u^h, and the flux is linear in K.

Now,

$$\omega_i = \varphi_i + \begin{cases} \sum_{K, i\in K}\gamma_i^K b^K & \text{if } x \in \text{ support of } \varphi \\ 0 & \text{else} \end{cases} \tag{10}$$

is *a continuous function* so that it can be used in the variational formulation.

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Denoting by $W_h = \text{span}(\omega_i)$ and $V_h = \text{span}(\varphi_i)$, the variational formulation of the problem is the following (we omit the boundary conditions (BC) for short and use some abuses of language): find $u^h \in V^h$ such that for all $w \in W_h$,

$$-\int_\Omega f^h(u^h)\cdot\nabla w\,\mathrm{d}K + \int_\Omega \varepsilon\nabla u^h\cdot\nabla w\,\mathrm{d}K = 0.$$

Setting $w = \omega_i$ the previous equation, and integrating by parts, the first term we obtain is

$$\sum_{K,i\in K}\int_K \left(\omega_i\nabla\cdot f^h(u^h) + \varepsilon\nabla u^h\cdot\nabla\omega_i\right)\mathrm{d}K.$$

The first term gives back $\beta_i^K\phi^K$. Let us have a look at the second one,

$$\int_K \nabla\omega_i\cdot\nabla u^h\,\mathrm{d}K = \int_K \nabla\varphi_i\cdot\nabla u^h\,\mathrm{d}K + \gamma_i^K\int_K \nabla b^K\cdot\nabla u^h\,\mathrm{d}K.$$

Since ∇u^h is constant, we see that

$$\int_K \nabla b^K\cdot\nabla u^h\,\mathrm{d}K = \nabla u^h\cdot\int\nabla b^K\,\mathrm{d}K,$$

and by the Green formula (which holds due to the continuity of b^K),

$$\int_K \nabla b^K\,\mathrm{d}K = \int_{\partial K} b^K\vec{n}\,\mathrm{d}K = 0.$$

This shows that the variational formulation is the following: find u^h such that for any i,

$$\sum_{K\ni i}\beta_i^K\phi^K + \varepsilon\int_K\nabla\varphi_i\cdot\nabla u\,\mathrm{d}K = 0,$$

that is, the RD scheme on the convection *plus* Galerkin on the diffusion. This is the argument used in [16] to justify the consistency of the aforementioned scheme. The method, however, does not show a uniform accuracy. This is a well-known problem of the Streamline Upwind Petrov Galerkin scheme that is recovered here with $\beta_i = \frac{1}{3} + k_i\tau$. One has to blend the scheme with a Galerkin approximation, the blending parameter depends on a cell Peclet number, see [11, 21] for details on the streamline method and the RD schemes.

How can we extend this to higher orders? The key argument here was that the gradient or the divergence of a linear field is constant, which is only true for linear triangular elements.

4. EXTENSION TO HIGHER DEGREES

The purpose of this section is to investigate whether or not the technique of the previous section can be extended to higher than second-order accurate schemes, in other words, to see whether or not the schemes described in [20] can be re-interpreted in a classical variational formulation with continuous test functions. We shall see that the answer is no.

We still assume $\mathbf{D} = \varepsilon\,\mathrm{Id}$. We want to find functions $\gamma_i^K \in H^1(K)$ such that

1. When we use a $\mathbb{P}^k$ Lagrange interpolant,

$$\int_K \left(\varphi_i + \gamma_i^K\right)\nabla\cdot f(u^h)\mathrm{d}K = \beta_i^K\int_K\nabla\cdot f(u^h)\,\mathrm{d}K. \tag{11a}$$

2. They enable to construct H^1 basis functions:

$$\left(\gamma_i^K\right)_{|\partial K} = 0. \tag{11b}$$

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3. They play no role on the viscous terms:

$$\int_K \gamma_i^K \Delta u \, \mathrm{d}K = \int_K \mathrm{div}\ \left(\gamma_i^K \nabla u\right)\ \mathrm{d}K - \int_K \nabla \gamma_i^K \cdot \nabla u \, \mathrm{d}K = 0,$$

that is, because $\left(\gamma_i^K\right)_{|\partial K} = 0$,

$$\int_K \nabla \gamma_i^K \cdot \nabla u \, \mathrm{d}K = 0 \tag{11c}$$

for any $u \in \mathbb{P}^k(K)$.

We can rephrase (11a) as

$$\int_K \gamma_i^K \nabla \cdot f(u^h) \, \mathrm{d}K = \beta_i^K \int_K \nabla \cdot f(u^h) \, \mathrm{d}K - \int_K \varphi_i \nabla \cdot f(u^h) \, \mathrm{d}K. \tag{12}$$

If the flux f is linear in u^h, the conditions (12)-(11b)-(11c) are affine conditions of the type

$$\ell_p\left(\gamma_i^K\right) = a_p,$$

where the linear functional ℓ_p are defined by the following:

1. From condition (12)

$$\ell_p^1(w) = \int_K w \nabla \cdot f(u^h) \, \mathrm{d}K,$$

and

$$a_p = \beta_i^K \int_K \nabla \cdot f(u^h) \, \mathrm{d}K - \int_K \varphi_i \nabla \cdot f(u^h) \, \mathrm{d}K,$$

2. From condition (11c)

$$\ell_p^2(w) = \int_K \nabla w \cdot \nabla u^h \, \mathrm{d}K$$

and $a_p = 0$.

Unfortunately, there is no solution to this problem, in general. Consider the simple 1D case, with quadratic elements. Any element can be mapped onto $[0, 1]$, so we can assume $K = [0, 1]$. In the case of quadratic and $f(u) = u$ elements, the Lagrange points are $\xi = 0$, $1/2$, and 1, and thus the Lagrange functions are

$$\varphi_0(x) = (1 - 2x)(1 - x), \quad \varphi_{1/2}(x) = 4x(1 - x), \quad \varphi_1(x) = x(2x - 1),$$

hence

$$\varphi_0'(x) = 4x - 3, \quad \varphi_{1/2}'(x) = 4 - 8x, \quad \varphi_1'(x) = 4x - 1.$$

By abuse of language, the functions γ_i^K and the coefficients β_i^K are now denoted by γ_ξ and β_ξ.

Since the second derivative of quadratic functions are constant, with the simplifications given by (11c), we obtain $\int_0^1 \gamma_\xi \mathrm{d}K = 0$. Using these expressions of φ_0', φ_1', and $\varphi_{1/2}'$ and this relation, (12) becomes

$$\varphi_0' : \qquad 4\int_0^1 \gamma_\xi x \mathrm{d}x = -\beta_\xi - \int_0^1 \varphi_\xi \varphi_0'(x) \mathrm{d}K, \tag{13a}$$

$$\varphi_{1/2}' : \qquad -8\int_0^1 \gamma_\xi x \mathrm{d}x = -\int_0^1 \varphi_\xi \varphi_{1/2}'(x) \mathrm{d}x, \tag{13b}$$

$$\varphi_1' : \qquad 4\int_0^1 \gamma_\xi x \mathrm{d}x = \beta_\xi - \int_0^1 \varphi_\xi \varphi_1'(x) \mathrm{d}x. \tag{13c}$$

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If one takes $\xi = 1/2$, we see (from (13b)) that $\int_0^1 \gamma_\xi x \mathrm{d}x = 0$, that is, $\beta_{1/2}$ is a given *fixed* constant and moreover independent of the scheme[¶]. This already suffices to show that we cannot, in general, build γ_i^K for any given scheme.

Let us show that, in general, β_ξ can be arbitrary in $[0, 1]$. To show that, we consider the limited scheme constructed from the Lax–Friedrichs scheme,

$$\phi_\xi = \frac{1}{3}(u_1 - u_0) + \alpha(u_\xi - \bar{u}) \text{ with } \bar{u} = \frac{1}{3}(u_0 + u_{1/2} + u_1).$$

We introduce

$$p = \frac{u_{1/2} - u_0}{u_1 - u_0} \text{ and } q = \frac{u_1 - u_{1/2}}{u_1 - u_0}.$$

We have $p + q = 1$; p can be arbitrary in $\mathbb{R}$. We define the ratios

$$x_0 = \frac{\phi_0}{\phi} = \frac{1}{3} - \alpha\frac{p+1}{3}, \quad x_{1/2} = \frac{\phi_{1/2}}{\phi} = \frac{1}{3} + \alpha\frac{p-q}{3}, \quad x_1 = \frac{\phi_{1/2}}{\phi} = \frac{1}{3} + \alpha\frac{q+1}{3}.$$

If $\alpha = 1$, we have some simplifications

$$x_0 = -\frac{p}{3}, \quad x_{1/2} = \frac{2}{3}p, \quad x_1 = \frac{3-p}{3}.$$

We see that if $p \in [0, 3]$, we obtain

$$\beta_0 = 0, \quad \beta_{1/2} = \frac{2p}{3+p} \quad \beta_1 = \frac{3-p}{3+p}.$$

We note that the image of $[0, 3]$ by $p \mapsto \frac{2p}{3+p}$ is $[0, 1]$; that is, the range of $\beta_{1/2}$ is at least $[0, 1]$, which is in contradiction to the fact that $\beta_{1/2}$ is the fixed given constant.

This shows that there is no solution to the problem in general and that something else must be carried out.

5. APPROXIMATION OF (1): VARIATIONAL METHODS BASED ON GRADIENT RECONSTRUCTION

We start again from the formulation (7)-(9). Taking $v^h \in V^h$, we have

$$\sum_i v_i^h \left(\sum_{K \ni i} \phi_i^K + \sum_{\Gamma \ni i} \phi_i^\Gamma \right) = \sum_K \left(\sum_{j \in K} \beta_j^K v_j^h \right) \int_{\partial K} f(u^h) \cdot \vec{n} \mathrm{d}\partial K + \sum_\Gamma \left(\sum_{j \in \Gamma} \beta_j^K v_j^h \right) \int_\Gamma \left(f(u^h) \cdot \vec{n} - \hat{f}(u^h, g, \vec{n}) \right) \mathrm{d}\partial K.$$

We introduce W^h the space of the functions that are piecewise constant on the elements K and the mapping

$$\pi_\beta^h : V^h \to W^h$$
$$v^h \mapsto \pi_\beta^h(v^h), \text{for all } K, \pi_\beta^h(v^h)_{|K} = \sum_{j \in K} \beta_j^K v_j^h.$$

In this definition, β stands for the set $\left\{\beta_j^K\right\}_{K, j \in K}$. In the following, β may depend on u^h, or more generally on some element $w^h \in V^h$ because the coefficients β_j^K may depend on w^h, so we write

[¶]In fact, the unique solution is $\beta_{1/2} = 1/4$.

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$\beta(w^h)$ or simply β if there is no ambiguity. The dependancy of β with respect to w^h is described later in this section.

We can reformulate the RD scheme as finding $u^h \in V^h$ such as for any $v^h \in V^h$,

$$a(u^h, v^h; u^h) = 0$$

with

$$a(u^h, v^h; w^h) := \sum_K \left(\int_{\partial K} \pi^h_{\beta(w^h)}(v^h) f(u^h) \cdot \vec{n} \mathrm{d}\partial K - \int_K \nabla \pi^h_{\beta(w^h)}(v^h) \cdot f(u^h) \mathrm{d}K \right). \quad (14)$$

We note that the exact solution u, if it is smooth enough, of (1) also satisfies the residual condition

$$a(u, v^h; w^h) = 0$$

for any $v^h, w^h \in V^h$. Indeed, in that case, we can also write

$$\sum_K \int_K \pi^h_{\beta(w^h)}(v^h) \mathrm{div}\ f(u) \mathrm{d}K = 0.$$

To derive the formulation for the viscous problem (1), $\mathbf{D} \not\equiv 0$, we start from that relation. If u is the solution of (1), it is known that it is a smooth function, and we can write for the continuous problem

$$\sum_K \int_K \pi^h_{\beta(w^h)}(v^h) \left[\mathrm{div}\ (f(u) - \mathbf{D}\nabla u) \right] \mathrm{d}K = 0.$$

By standard calculations, we obtain

$$\sum_K \int_{\partial K} \pi_h(w^h) f(u) \cdot \vec{n} \mathrm{d}K + \int_{\partial K} \pi_h(w^h) (\mathbf{D}\nabla u) \cdot \vec{n} \mathrm{d}\partial K = 0.$$

Since $(\mathbf{D}\nabla u) \cdot \vec{n}$ is continuous across any edge of $\mathcal{T}_h$ for a smooth enough solution, and using some average operator,[‖] we can equivalently rewrite this relation as

$$\sum_K \int_{\partial K} \pi_h(v^h) f(u) \cdot \vec{n} \mathrm{d}K + \int_{\partial K} \pi_h(w^h) \{(\mathbf{D}\nabla u) \cdot \vec{n}\} \mathrm{d}\partial K = 0^{**} \quad (15)$$

and consider the variational formulation that takes into account the boundary conditions as in (1)

$$\begin{aligned} \sum_K \Bigg\{ & \int_{\partial K} \pi^h_\beta(v^h) f(u) \cdot \vec{n} \mathrm{d}\partial K + \int_{\partial K} \pi^h_\beta(v^h) \{(\mathbf{D}\nabla u) \cdot \vec{n}\} \mathrm{d}\partial K \\ & + h_K \int_K \left(\nabla_u f(u^h) \cdot \nabla v^h - \nabla \cdot (\mathbf{D}\nabla v^h) \right) \left(\nabla_u f(u^h) \cdot \nabla u^h - \nabla \cdot (\mathbf{D}\nabla u^h) \right) \mathrm{d}K \Bigg\} \quad (16) \\ & + \sum_{\Gamma \subset \Gamma_W} \int_\Gamma \pi^h_\beta(v^h) \left(f(u^h) \cdot \vec{n} - \hat{f}(u^h, g_w, \vec{n}) \right) \mathrm{d}\Gamma = 0. \end{aligned}$$

In (16), we have made the following assumptions:

1. The mesh is adapted to the boundary conditions. In particular, the union of the boundary edges on Γ_W is Γ_W exactly. This also means that Ω has a polygonal shape. The more general case can be handled via isoparametric approximation as in [20, 22].

[‖] In fact, we can use any consistent average that is equal to $D\nabla u \cdot \vec{n}$ when the normal flux $D\nabla u \cdot n$ is continuous accross that edge.

[**] The matrix $\mathbf{D}$ may depend on u, ∇u, and so forth.

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2. u^h and the test functions v^h are respectively sought for in the functional spaces

$$V_h = \left\{ u^h \text{ continuous and defined on } \Omega, u_K^h \in \mathbb{P}^k(K) \text{ for any element K and } u^h_{|\Gamma_S} = gs \right\}$$
$$V_h' = \left\{ v^h \text{ continuous and defined on } \Omega, v_K^h \in \mathbb{P}^k(K) \text{ for any element K and } u^h_{|\Gamma_S} = 0 \right\}$$

The choice of β is free, we choose it so that the convective operator, without the filtering operator, leads to a maximum principle satisfying scheme. To achieve this, in each K, we proceed as follows:

1. We consider the Lax–Friedrichs residual. For any degree of freedom in K,

$$\phi_\sigma^{\mathrm{LLF},K} = \frac{1}{N_K} \int_{\partial K} \left(f(u^h) \cdot \vec{n} - \{ \mathbf{D} \nabla u \cdot \vec{n} \} \right) \mathrm{d}\partial K + \alpha_K (u_\sigma - \overline{u}_K)$$

   where α_K is a bound of $|\nabla_u f|$ on K, N_K the number of degrees of freedom in K and

$$\overline{u}_K = \frac{1}{N_K} \sum_{\sigma \in K} u_\sigma, \tag{17}$$

2. β_σ^K is evaluated from

$$\beta_\sigma^K = \frac{\max\left(\frac{\phi_\sigma^{\mathrm{LLF},K}}{\phi^K}, 0 \right)}{\sum_{\sigma' \in K} \max\left(\frac{\phi_{\sigma'}^{\mathrm{LLF},K}}{\phi^K}, 0 \right)}, \tag{18}$$

   recall that

$$\phi^K = \int_{\partial K} \left(f(u^h) \cdot \vec{n} - \{ \mathbf{D} \nabla u \cdot \vec{n} \} \right) \mathrm{d}\partial K.$$

3. The average operator $\{ . \}$ has to be consistent. The next paragraph is devoted to the description of the reconstructions we have employed in this work.
4. We have added a filtering term similar to (6) but adapted to (1), namely

$$\Phi_\sigma^{K,\mathrm{F}} = \int_K \left(\nabla f_u \cdot \nabla \varphi_\sigma - \nabla \cdot (\mathbf{D} \nabla \varphi_\sigma) \right) \tau \left(\nabla f_u \cdot \nabla u - \nabla \cdot (\mathbf{D} \nabla u) \right) \mathrm{d}K. \tag{19}$$

The actual scheme writes

$$\Phi_\sigma^{\mathrm{LLFF}} = \beta_\sigma^K \phi^K + \Phi_\sigma^{K,\mathrm{F}}.$$

The acronym "LLFF" stands for "Local Lax–Friedrichs Filtered".

Remark 5.1
We can easily extend this to the case of discontinuous RD scheme, see [2, 3, 23].

5.1. Gradient reconstruction methods

We have considered techniques that reconstruct gradients using a L^2 projection and piecewise continuous polynomials. There are many possible choices depending on how are defined the degrees of freedom. An obvious choice is to project the gradient on the same space as the one we have used to approximate the solution. Hence, we write

$$\int_\Omega \varphi_\sigma \{\nabla u\} \, \mathrm{d}\Omega = \sum_{K, \sigma \in K} \int_K \varphi_\sigma \, \nabla u|_K \, \mathrm{d}K, \qquad \text{for any degree of freedom } \sigma \tag{20}$$

where

$$\{\nabla u\} = \sum_{\sigma \in \mathcal{T}_h} \varphi_\sigma \{\nabla u\}_\sigma \qquad \nabla u|_K = \sum_{\sigma \in K} u_\sigma \nabla \varphi_\sigma. \tag{21}$$

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The linear system defined by (20) is not diagonal, so the solution, although not difficult to obtain, is a bit expensive to proceed this way. It is possible to use mass lumping. To have an accuracy of order k if k is the polynomial degree, the weights are $1/3$ in the $\mathbb{P}^1$; $\left(\frac{1}{12}, \frac{1}{12}, \frac{1}{12}, \frac{3}{12}, \frac{3}{12}, \frac{3}{12}\right)$ (weights for the 3 vertices and 3 midpoints) in the $\mathbb{P}^2$ case. In both cases, the maximal accuracy on the gradient is met.

It is also possible to have exact mass lumping at the price of changing the approximation representation. Following [24, 25], we have tested enriched elements, initially built to allow mass lumping in Galerkin discretizations of time-dependent problems. For example, the $\mathbb{P}^{2+}$ triangle simply has one additional (with respect to the standard $\mathbb{P}^2$ triangle) degree of freedom that is located in its centroid (see Figure 1). Using the seven points of the enriched element, a quadrature formula exact for polynomials of degree 2 can be constructed. We refer to [24, 25] for details.

From the implementation point of view, from (21), we obtain

$$\{\nabla u\}_\sigma = \frac{\sum_{K,\sigma\in K} |K|\omega_\sigma \nabla u^h(\sigma)}{\sum_{K,\sigma\in K} |K|\omega_\sigma} \tag{22}$$

where the ω_σs are the weight associated to the quadrature formula. We note that, since only a maximal accuracy of order k can be met, we can also apply (22) with $\omega_\sigma = 1$ for any σ.

Anticipating a bit of the numerical section, none of the reconstruction shows definite superiority compared with the others; hence, we have privileged simplicity of implementation. This is why all the numerical examples are obtained with (22) with $\omega_\sigma = 1$ for any σ.

5.2. Dealing with the diffusion-dominated case

The LLFF scheme that used this reconstruction has the expected behavior for small values of the diffusion coefficients. However, when the cell Reynolds number $\|\nabla_u f\| h/\nu$ is moderate or small, the (grid) convergence rate obtained is considerably less than the $k+1$ value we aim at. When diffusion starts becoming important, the convergence curve suffers perturbations, and its rate decreases drastically. In a diffusion-dominated configuration, the scheme completely fails to converge.

To cure this flaw, we have blended the current limited LLFF scheme with a LW scheme obtained by rewriting the advection–diffusion problem as a system of first-order PDEs, as proposed in [13] and then in [15, 26]. In the diffusion-dominated case, the LW scheme nodal residuals writes

$$\Phi_\sigma^{\mathrm{LW}} = \frac{1}{N_K}\Phi^K + \mathbf{C}\int_K \nabla\varphi_\sigma \left(\nabla u^K - \{\nabla u\}\right) \mathrm{d}K\,, \quad \text{with } \Phi^K = -\int_{\partial K} \left\{\mathbf{D}\nabla u\cdot\vec{n}\right\} \mathrm{d}\partial K$$

where we set $\mathbf{C} = 0.5$ when working with triangles. As shown in [13], this term can be related to the least-square stabilization associated to the first-order system form of the equation. The LW scheme reaches respectively second and third order when solving the purely diffusive scalar equation using a $\mathbb{P}^1$ (respectively $\mathbb{P}^2$) formulation.

When solving the advection–diffusion equation, we blend the LLFF scheme with the LW scheme. The blending parameter is a function of the cell Reynolds number $\xi(Re)$. This function is computed

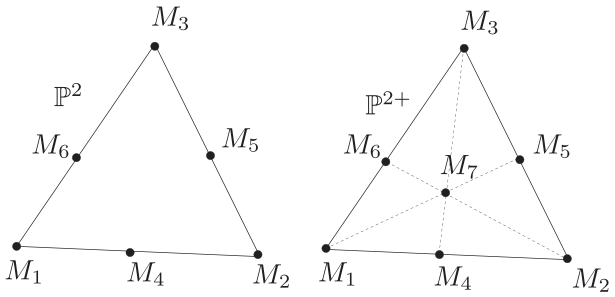

Figure 1. Standard $\mathbb{P}^2$ and enriched $\mathbb{P}^{2+}$ triangles

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following again [15, 26]. In practice, first we define a modified Lax–Friedrichs scheme, by turning off the Lax–Friedrichs dissipation in the purely diffusive regime, and apply the limiter as discussed before so that we obtain

$$\Phi_\sigma^{K,\text{LLF–LW}} = \frac{1}{N_K}\Phi^K + \xi(Re)\alpha^K\left(u_i - \overline{u}\right).$$

Then, we compute the limited residuals $\Phi_\sigma^{K,\text{LLF–LW}^*}$ following the procedure (18). We then add the least-squares term (19) in advection-dominated flows and the LW least-squares term in the diffusion-dominated one. The resulting scheme reads

$$\Phi_\sigma^{K,\text{LLFF–LW}^*} = \Phi_\sigma^{K,\text{LLF–LW}^*} + \xi(Re)\Phi_\sigma^{K,\text{F}} + (1-\xi(Re))\,\Phi_\sigma^{K,\text{LW}}. \tag{23}$$

The parameter $\xi(Re)$ that we have used in effective calculations is

$$\xi(Re) = \max\left(0, 1 - \frac{1}{Re}\right). \tag{24}$$

In terms of CPU cost, computing the LW integral term is not very demanding. The same quadrature formula used for the reconstruction, using only the element's degrees of freedom, has proven to be enough to provide the best convergence rates achievable with this approach. In particular, on $\mathbb{P}^2$ elements, the blended scheme reaches third order at both limits but is still experiencing a precision loss around $Re \sim 1$ (cf. Section 6). Similar conclusions are obtained when using both standard $\mathbb{P}^2$ and enriched $\mathbb{P}^{2+}$ elements.

The choice (24) is such that the diffusive/advection limits of the scheme is reached much before it is the case in the continuous system. This allows to get rid of the computation cost of one of the stabilization terms. In particular, when facing a pure diffusive flow configuration, cutting out the cost associated to the LLFF scheme results in a critical speed-up. In practice, when the Reynolds based function comes close enough from its bounds (0 and 1), we force it to take the limit value. This is obtained by defining the modified blending function.

6. NUMERICAL ILLUSTRATIONS

We present two test cases. The first one is an accuracy test. In the second case, we check the nonoscillatory properties of the scheme.

6.1. Grid convergence on a truly 2D problem

We are solving (1) on $\Omega = [0,1]^2$, with

$$f(u) = \frac{\sqrt{2}}{2}\begin{pmatrix} 1 \\ -1 \end{pmatrix} u \text{ and } D = \varepsilon \text{Id}.$$

The Dirichlet conditions are set such that the exact solution is

$$U_{\text{ex}}(x,y) = -\cos(2\pi\eta)\exp\left[\frac{1}{2\varepsilon}\xi\left(1-\sqrt{1+(4\pi\varepsilon)^2}\right)\right] \text{ in } [0,1]^2$$
$$\xi = \cos\left(\frac{\pi}{4}\right)x + \sin\left(\frac{\pi}{4}\right)y,$$
$$\nu = \sin\left(\frac{\pi}{4}\right)x - \cos\left(\frac{\pi}{4}\right)y,$$

that is, g is the restriction of U_{ex} on $\partial\Omega$.

For several values of the parameter ε, we have conducted a convergence study that uses eight triangulated meshes, with mesh sizes from $h \approx 1/10$ to $h \approx 1/80$. The study covers a wide range of flow configurations: diffusion-dominated ($\log(Re) \ll 0$), advection–diffusion ($\log(Re) \approx 0$), and advection-dominated ($\log(Re) \gg 0$). We compare three numerical schemes, all using the reconstructed gradients approach. The first one is the $\mathbb{P}^2$ LLFF scheme, the second one is the $\mathbb{P}^2$

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Table I. Results obtained with the LLFF $\mathbb{P}^2$ scheme, then with the LLFF–LW* $\mathbb{P}^2$ scheme and finally with the $\mathbb{P}^{2+}$ enriched element version.

		LLFF		LLFF–LW*		LLFF–LW* ($\mathbb{P}^{2+}$)	
				$\varepsilon = 1$			
$\log_{10}(Re)$	$\log_{10}(h)$	$\log_{10}$ of the L^2 error	Order	$\log_{10}$ of the L^2 error	Order	$\log_{10}$ of the L^2 error	Order
−1.01	−1.01	−2.58	–	−3.76	–	−3.66	–
−1.31	−1.31	−3.06	1.59	−4.73	3.22	−4.42	2.52
−1.49	−1.49	−3.33	1.58	−4.928	2.56	−4.80	2.38
−1.62	−1.62	−3.39	1.34	−5.37	2.66	−5.28	2.68
−1.71	−1.71	x	x	−5.65	2.70	−5.54	2.69
−1.79	−1.79	x	x	−5.99	2.87	−5.88	2.86
−1.86	−1.86	x	x	−6.23	2.92	−5.98	2.74
−1.92	−1.92	x	x	−6.36	2.88	−6.14	2.75
				$\varepsilon = 0.01$			
$\log_{10}(Re)$	$\log_{10}(h)$	$\log_{10}$ of the L^2 error	Order	$\log_{10}$ of the L^2 error	Order	$\log_{10}$ of the L^2 error	Order
0.99	−1.01	−2.36	–	−2.46	–	−2.31	–
0.69	−1.31	−3.06	2.31	−3.13	2.21	−3.26	3.14
0.51	−1.49	−3.47	2.33	−3.49	2.16	−3.59	2.68
0.38	−1.62	−3.73	2.27	−3.73	2.10	−3.81	2.48
0.29	−1.71	−3.91	2.22	−3.93	2.09	−3.98	2.39
0.21	−1.79	−4.02	2.14	−4.07	2.07	−4.11	2.32
0.14	−1.86	−4.10	2.05	−4.20	2.06	−4.25	2.30
0.08	−1.92	−4.18	2.01	−4.32	2.06	−4.37	2.28
				$\varepsilon = 0.0001$			
$\log_{10}(Re)$	$\log_{10}(h)$	$\log_{10}$ of the L^2 error	Order	$\log_{10}$ of the L^2 error	Order	$\log_{10}$ of the L^2 error	Order
2.99	−1.01	−2.90	–	−2.94	–	−2.85	–
2.69	−1.31	−3.81	3.00	−3.83	2.95	−3.72	2.89
2.51	−1.49	−4.36	3.05	−4.37	3.01	−4.26	2.96
2.38	−1.62	−4.70	2.98	−4.71	2.94	−4.62	2.93
2.29	−1.71	−4.99	2.99	−5.00	2.95	−4.91	2.94
2.21	−1.79	−5.21	2.97	−5.22	2.93	−5.12	2.92
2.14	−1.86	−5.40	2.96	−5.41	2.93	−5.30	2.90
2.08	−1.92	−5.58	2.96	−5.59	2.93	−5.48	2.91

LLFF, Local Lax–Friedrichs Filtered; LW, Lax–Wendroff

LLFF–LW*, and the last one is the $\mathbb{P}^{2+}$ LLFF–LW*. The results of these mesh convergence studies are presented in Table I.

We first note that the LLFF scheme experiences convergence problems in the case of the diffusion-dominated configuration ($\varepsilon = 1$). The test stops at the fourth mesh for this scheme. The achieved order of accuracy is close to 3 in the advection-dominated configuration and decreases to 2 when $\log(Re) \approx 0$.

The LLFF–LW* formulation behaves exactly as the LLFF scheme for both advection–diffusion and advection-dominated flows, respectively achieving a precision of 2 and 3. The LW blending improves the convergence of the scheme in the diffusion-dominated case where third-order accuracy is now achieved.

The $\mathbb{P}^{2+}$ formulation of the LLFF–LW* scheme slightly improves the results in the advection–diffusion case, in which we achieve convergence rates larger than 2 (between 2.3 and 3) but still far from optimal and uniform. It is not clear that this minor improvement is worth the additional cost of the extra degree of freedom.

6.2. Resolution of steep gradients

We are interested in solving the Smith and Hutton problem

$$\begin{aligned} &\operatorname{div}(\vec{\lambda} u) - \varepsilon \Delta u = 0 \quad && x \in \Omega \\ &u = g && \text{on } \partial\Omega \end{aligned}$$

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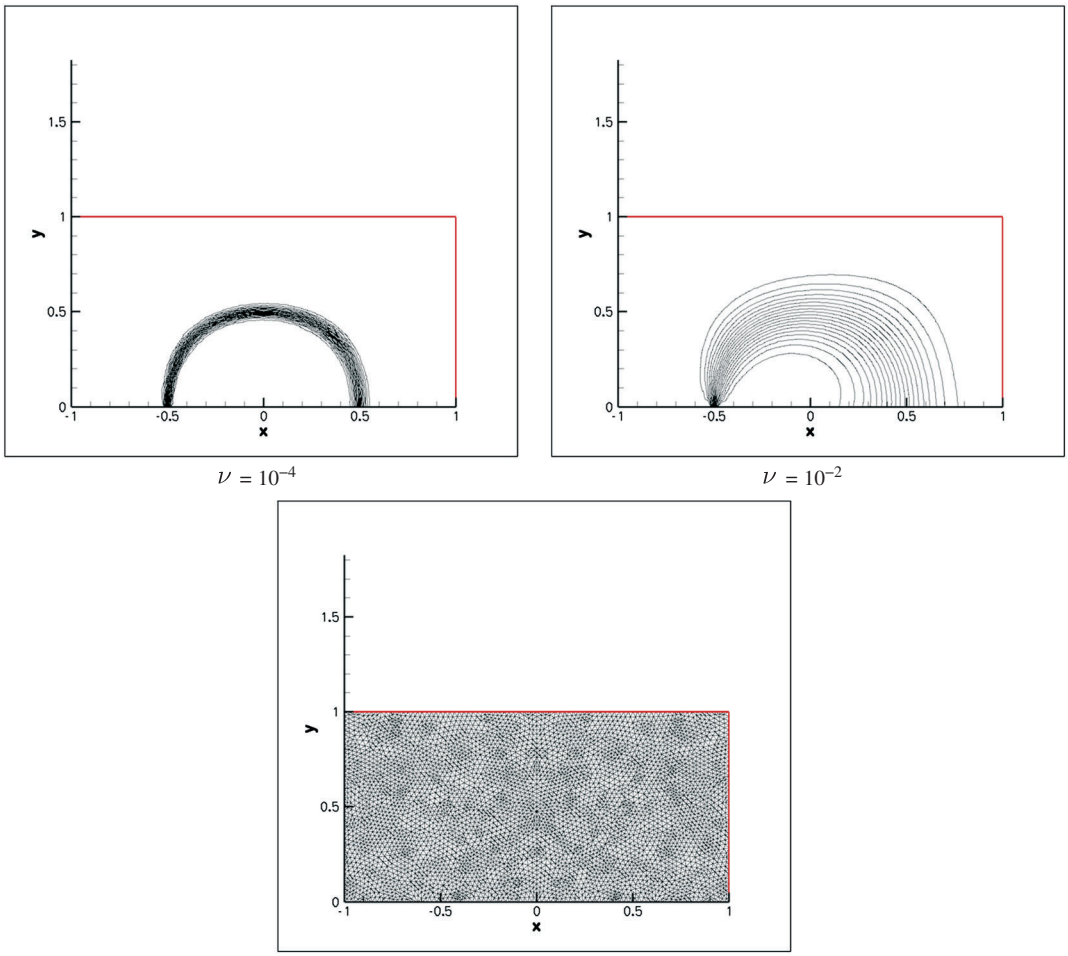

$\nu = 10^{-4}$ $\nu = 10^{-2}$

Mesh (all the degrees of freedom are displayed)

Figure 2. Smith and Hutton case with $\alpha = 100$ for different viscosities.

with

$$\vec{\lambda} = (2y(1-x^2), -2x(1-y^2))^T, \quad \Omega = [-1,1] \times [0,1],$$
$$f = 0 \qquad \text{and } g(x,y) = 1 + \tanh\left(\delta(1 - 2\sqrt{\psi})\right),$$

$\psi(x,y) = 1 - (1-x^2)(1-y^2)$ and $\delta = 100$. The usual choice for δ is 10, resulting is much less steep gradients. This case enables to check the ability of the LLFF–LW* scheme to handle very steep solution gradients. As shown in Figure 2, no particular problem are encountered. There is no known analytical formula for this problem; hence, it is not possible to conduct a convergence study.

7. CONCLUSION, FUTURE WORK

We have explored several discretization of the steady convection–diffusion (1) by means of RD schemes. These schemes degenerate to standard RD schemes when the diffusion effects vanish and are nonoscillatory. We have first shown that the method used in the case of triangular linear element cannot be extended to more general case. It can be shown that the scheme is still consistent (see [27]), but one cannot reach optimal accuracy. Thanks to a reformulation of the inviscid RD scheme as a variational formulation, we can rely on this reformulation to develop a class of

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schemes adapted to (1). They need a gradient reconstruction, and several options are studied. Several numerical simulations are carried out and demonstrated the expected accuracy, at least from moderate to high local Reynolds numbers.

These methods are being extended to the Navier–Stokes equations, see [28] for preliminary results.

APPENDIX A: IMPLEMENTATION REMARK

One of the difficulty of the scheme using reconstruction is that one needs to evaluate

$$\int_K \left(\nabla_u f(u^h)\cdot\nabla v^h - \nabla(\mathbf{D}\nabla v^h)\right)\left(\nabla_u f(u^h)\cdot\nabla u^h - \nabla(\mathbf{D}\nabla u^h)\right)\mathrm{d}x.$$

This is carried out by using the same trick as in [19] to reduce the number of arithmetic operations. The quadrature points are some of the Lagrange points. The second difficulty is to evaluate $\nabla(\mathbf{D}\nabla u^h)$. To do this, we notice that if $u^h \in \mathbb{P}^k(K)$, then $\nabla u^h \in \mathbb{P}^{k-1}(K)$, so that

$$\nabla u^h = \sum_{\sigma\in K} \nabla u^h(\sigma)\varphi_\sigma$$

where the φ_σ are the Lagrange basis functions. Then, $\mathbf{D}\nabla u^h$ is approximated with the right order by

$$\mathbf{D}\nabla u^h \approx \sum_{\sigma\in K}\left(\mathbf{D}\nabla u^h\right)(\sigma)\varphi_\sigma.$$

To evaluate pointwise $\nabla(\mathbf{D}\nabla u^h)$, it is enough to apply twice the algorithm to evaluate the gradient.

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