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Volker John and Ellen Schmeyer

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Volker John

Saarland University
Department of Mathematics
P.O. Box 15 11 50
66041 Saarbrücken
Germany
john@math.uni-sb.de

Ellen Schmeyer

Saarland University
Department of Mathematics
P.O. Box 15 11 50
66041 Saarbrücken
Germany
schmeyer@math.uni-sb.de

Edited by
FR 6.1 – Mathematik
Universität des Saarlandes
Postfach 15 11 50
66041 Saarbrücken
Germany

Fax: + 49 681 302 4443
e-Mail: preprint@math.uni-sb.de
WWW: http://www.math.uni-sb.de/

Abstract

The paper studies finite element methods for the simulation of time–dependent convection–diffusion–reaction equations with small diffusion: the SUPG method, a SOLD method and two types of FEM–FCT methods. The methods are assessed, in particular with respect to the size of the spurious oscillations in the computed solutions, at a 3D example with nonhomogeneous Dirichlet boundary conditions and homogeneous Neumann boundary conditions.

1 Introduction

The simulation of various applications requires the numerical solution of time–dependent convection–diffusion–reaction equations. A typical example are processes which involve a chemical reaction in a flow field [5]. Such a reaction can be modeled with a coupled system of time–dependent nonlinear convection–diffusion–reaction equations for the concentrations of the reactants and the products.
Typically, the solution of these equations possesses layers. A numerical method for the simulation of these equations, whose results can be considered to be useful, should meet two requirements:

- sharp layers (with respect to the used mesh size) should be computed,
- spurious oscillations in the solution must not occur.

The second requirement means in particular that the computed solution does not have negative values if, for instance, the behavior of concentrations is simulated. A number of finite element methods have been developed for the simulation of convection–diffusion–reaction equations with small diffusion. One of the most popular ones is the streamline upwind Petrov–Galerkin (SUPG) method from [2, 1]. This method leads to solutions with sharp layers, however also with sometimes considerable spurious oscillations. To reduce these oscillations, a number of so–called Spurious Oscillations at Layers Diminishing (SOLD) schemes have been proposed, see the reviews [3, 4]. SOLD schemes add additional, in general nonlinear, stabilization terms to the SUPG method. A completely different finite element approach of treating equations with small diffusion are Finite Element Method Flux–Corrected–Transport (FEM–FCT) schemes [10, 8]. These methods do not modify the bilinear form but they manipulate the matrix and the right hand side of a Galerkin finite element method.
A first comparison of finite element methods for time–dependent convection–diffusion–reaction equations was presented in [6]. The numerical examples of

[6] studied problems in 2D with homogeneous Dirichlet boundary conditions. The present paper extends the studies of [6] to 3D problems with inhomogeneous Dirichlet and Neumann boundary conditions. This is a realistic situation in applications.

2 Finite element methods time–dependent convection–diffusion–reaction equations

We consider a linear time–dependent convection–diffusion–reaction equation

$$u_t - \varepsilon\Delta u + \mathbf{b}\cdot\nabla u + cu = 0 \quad \text{in } (0,T]\times\Omega, \tag{1}$$

where $\varepsilon > 0$ is the diffusion coefficient, $\mathbf{b} \in L^\infty(0,T;(W^{1,\infty}(\Omega)))$ is the convection field, $c \in L^\infty(0,T;L^\infty(\Omega))$ is the non–negative reaction coefficient, $T > 0$ is the final time and $\Omega \subset \mathbb{R}^3$ is a bounded domain. This equation has to be equipped with an initial condition $u_0 = u(0,\mathbf{x})$ and with appropriate boundary conditions.
In the numerical studies, (1) will be discretized in time with the Crank-Nicolson scheme using equidistant time steps Δt. This leads in the discrete time t_k to the equation

$$\begin{aligned} & u_k + 0.5\Delta t\left(-\varepsilon\Delta u_k + \mathbf{b}\cdot\nabla u_k + cu_k\right) \\ &= u_{k-1} - 0.5\Delta t\left(-\varepsilon\Delta u_{k-1} + \mathbf{b}\cdot\nabla u_{k-1} + cu_{k-1}\right) + 0.5\Delta t f_{k-1} + 0.5\Delta t f_k. \end{aligned} \tag{2}$$

Equation (2) can be considered as a steady–state convection–diffusion–reaction equation, with the diffusion, convection and reaction, respectively, given by

$$D = 0.5\Delta t\varepsilon, \quad \mathbf{C} = 0.5\Delta t\mathbf{b}, \quad R = 1 + 0.5\Delta t c.$$

The Galerkin finite element method reads as follows: Find $u_k^h \in V_{\text{ans}}^h$ such that

$$\begin{aligned} & (u_k^h, v^h) + 0.5\Delta t\left((\varepsilon\nabla u_k^h, \nabla v^h) + (\mathbf{b}\cdot\nabla u_k^h + cu_k^h, v^h)\right) \\ &= (u_{k-1}^h, v^h) - 0.5\Delta t\left((\varepsilon\nabla u_{k-1}^h, \nabla v^h) + (\mathbf{b}\cdot\nabla u_{k-1}^h + cu_{k-1}^h, v^h)\right) \\ &\quad + 0.5\Delta t(f_{k-1}, v^h) + 0.5\Delta t(f_k, v^h) \end{aligned} \tag{3}$$

for all V_{test}^h, where V_{ans}^h and V_{test}^h are appropriate finite element spaces.
The SUPG method adds a consistent diffusion term in streamline direction to the left hand side of (3)

$$\sum_{K\in\mathcal{T}^h} \tau_K \left(R^h(u_k^h), \mathbf{C}\cdot\nabla v^h\right)_K,$$

where $\{\tau_K\}$ is a set of parameters depending on the mesh cells $\{K\}$. The residual $R^h(u_k^h)$ is defined by the difference of the left hand side and the right hand side of (2). Different proposals for the choice of the parameters $\{\tau_K\}$ can be found in the literature. In the numerical studies of [6], the choice from [7]

$$\tau_K = \min\left\{\frac{h_K}{\Delta t\|\mathbf{b}\|_2}, \frac{1}{1+0.5\Delta t c}, \frac{2h_K^2}{\Delta t\varepsilon}\right\},$$

where $\|\cdot\|_2$ denotes the Euclidean norm of a vector, has been proven to be the best one. However, it is well known that numerical solutions which are computed with the SUPG method often possess non–negligible spurious oscillations at the layers.

SOLD methods are trying to reduce the spurious oscillations of SUPG methods by adding another stabilization term to the SUPG method. This stabilization term is in general nonlinear. There are several classes of SOLD methods, see [3, 4]. It was found in the numerical studies of [6] that the best results among the SOLD methods were obtained with a method adding an anisotropic diffusion term

$$(\tilde{\varepsilon}\mathbb{C}_{\text{os}}\nabla u_k^h, \nabla v^h) \quad \text{with} \quad \mathbb{C}_{\text{os}} = \begin{cases} I - \dfrac{\mathbf{C}\otimes\mathbf{C}}{\|\mathbf{C}\|_2^2} & \text{if } \mathbf{C}\neq\mathbf{0}, \\ 0 & \text{else,} \end{cases}$$

and the parameter

$$\tilde{\varepsilon}|_K = \max\left\{0, C\frac{\text{diam}(K)|R^h(u_k^h)|}{2\|\nabla u_k^h\|_2} - D\right\}, \tag{4}$$

where $\text{diam}(K)$ is the diameter of a mesh cell K. This type of parameter was proposed in [7] and modified to the form (4) in [3]. The SOLD parameter (4) contains a free parameter C which has to be chosen by the user.

The last approach which will be studied in our numerical tests are FEM–FCT schemes. They start with the algebraic equation which corresponds to the Galerkin finite element method (3)

$$(M_C + 0.5\Delta t A)u_k = (M_C - 0.5\Delta t A)u_{k-1} + 0.5\Delta t f_{k-1} + 0.5\Delta t f_k, \tag{5}$$

where $(M_C)_{ij} = (m_{ij}) = (\varphi_j, \varphi_i)$ is the consistent mass matrix. The first goal of FEM–FCT schemes consists in manipulating (5) such that a stable but low order scheme is represented. To this end, define $L = A + D$ with

$$D = (d_{ij}), \quad d_{ij} = -\max\{0, a_{ij}, a_{ji}\} = \text{for } i\neq j,\ d_{ii} = -\sum_{j=1, j\neq i}^{N} d_{ij},$$

and $M_L = \mathrm{diag}(m_i)$ with $m_i = \sum_{j=1}^{N} m_{ij}$, where N is the number of degrees of freedom. M_L is called lumped mass matrix. The low order scheme reads

$$(M_L + 0.5\Delta t L)u_k = (M_L - 0.5\Delta t L)u_{k-1} + 0.5\Delta t f_{k-1} + 0.5\Delta t f_k. \qquad (6)$$

The second goal of FEM–FCT schemes consists in the modification of the right hand side of (6) such that diffusion is removed in (6) where it is not needed but spurious oscillations are still suppressed

$$\begin{aligned}(M_L + 0.5\Delta t L)u_k &= (M_L - 0.5\Delta t L)u_{k-1} + 0.5\Delta t f_{k-1} + 0.5\Delta t f_k \\ &\quad + f^*(u_k, u_{k-1}). \qquad (7)\end{aligned}$$

The computation of the anti–diffusive flux vector $f^*(u_k, u_{k-1})$ is somewhat involved and we refer to [8, 9, 10, 6] for details. Its computation relies on a predictor step which uses an explicit and stable low order scheme. Thus, a stability issue arises in FEM–FCT schemes which leads to the CFL–like condition $\Delta t < 2 \min_i m_i / l_{ii}$. This condition was fulfilled in the numerical tests presented in Section 3. We will consider a nonlinear approach for computing $f^*(u_k, u_{k-1})$ [10, 9] and a linear approach [8].

3 Numerical studies

We consider a situation which has some typical features of a chemical reaction in application. First, the domain is three dimensional, $\Omega = (0,1)^3$. There is an inlet at $(0, 5/8, 5/8) \times (0, 6/8, 6/8)$ and an outlet at $(1, 3/8, 4/8) \times (1, 4/8, 5/8)$. The convection is given by $\mathbf{b} = (1, -1/4, -1/8)^T$, which corresponds to the vector pointing from the center of the inlet to the center of the outlet. Thus, the convection will not be aligned to the mesh. The diffusion is given by $\varepsilon = 10^{-6}$ and the reaction by

$$c(\mathbf{x}) = \begin{cases} 1 & \text{if } \|\mathbf{x} - g\|_2 \leq 0.1 \\ 0 & \text{else,} \end{cases}$$

where g is the line through the center of the inlet and the center of the outlet. That means, a reaction takes place only where the solution (concentration) is expected to be transported. The inflow boundary condition is

$$u_{\text{in}} = \begin{cases} \sin(\pi t/2) & \text{if } t \in [0,1] \\ 1 & \text{if } t \in (1,2] \\ \sin(\pi(t-1)/2) & \text{if } t \in (2,3]. \end{cases}$$

At the outflow, homogeneous Neumann boundary conditions are prescribed. The right hand side was set to be $f = 0$ in Ω for all times and the final time

in our numerical studies was $T = 3$. The orders of magnitudes for diffusion, convection, reaction and concentration correspond to the situation of [5].
Results will be presented for the P_1 finite element on a tetrahedral mesh and the Q_1 finite element on a hexahedral mesh. The number of degrees of freedom on both meshes is 35 937, including Dirichlet nodes. The diameter of the mesh cells is about 0.054 for the hexahedral mesh and between 0.054 and 0.076 for the tetrahedral mesh. The Crank–Nicolson scheme was applied with $\Delta t = 0.001$.
From the construction of the problem, it is expected that the solution is transported from the inflow to the outflow with a little smearing due to the diffusion. It should take values in $[0, 1]$. The size of the spurious oscillations in the numerical schemes will be illustrated with $u^h_{\min}(t)$, Fig. 1, the size of the undershoots. The undershoots are particularly dangerous in applications since they represent non–physical situations, like negative concentrations. Fig. 2 shows the distribution of the undershoots with $u^h_{\min}(t) \leqslant 0.01$ for the SUPG method at $t = 2$. Cut planes of the solutions at $t = 2$ are given in Figs. 3 – 7. These cut planes contain the centers of the inlet and the outlet and they are parallel to the z–axis. Note, some wiggles which can be seen in the contour lines, might be due to the rather coarse meshes. For illustrating the spurious oscillations, a color bar is given for each cut plane.

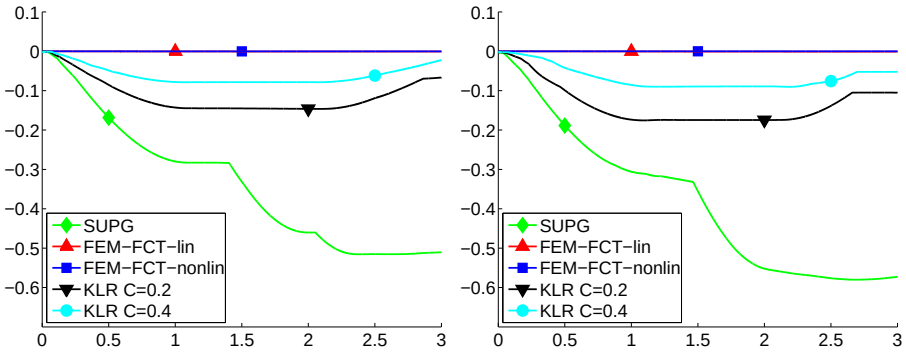

Figure 1: Minimal value of finite element solutions $u^h_{\min}(t)$, left Q_1, right P_1.

The numerical results show the large amount of spurious oscillations in the solutions computed with the SUPG method. Fig. 2 demonstrates that the solutions are globally polluted with spurious oscillations. The oscillations were considerably reduced and localized (not shown here) with the SOLD method KLR02. Increasing the constant leads to a decrease of the spurious oscillations, Fig 1. From the numerical studies of [3, 4] it is known that an increase of the constant results to somewhat more smearing of the solutions. However, this is rather tolerable in applications than spurious oscillations.

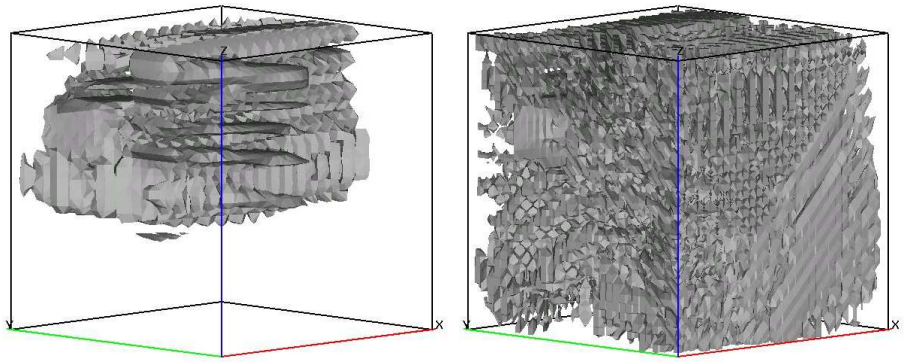

Figure 2: Distribution of negative oscillations $u^h_{\min}(t) \leqslant 0.01$ for the SUPG method at $t = 2$, left Q_1, right P_1.

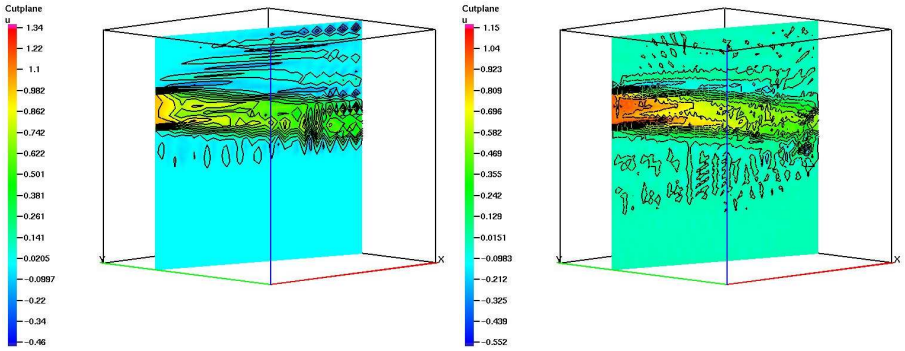

Figure 3: Cut of the solution, SUPG method at $t = 2$, left Q_1, right P_1.

The solutions obtained with the FEM–FCT methods are almost free of spurious oscillations. These schemes gave the best results in the numerical studies. Computing times for the methods are given in the Table 1. For solving the equations in the nonlinear schemes, the same fixed point iteration as described in [4, 6] was used. The iterations were stopped if the Euclidean norm of the residual was less than 10^{-8}. It can be observed that the nonlinear schemes are considerably more expensive than the linear methods. In KLR02, the computing times increase with increasing size of the user–chosen parameter. All observations correspond to the results obtained in [6] for 2D problems.

4 Summary and Conclusions

The paper studied several finite element method for solving time–dependent convection–diffusion–reaction equations in a 3D domain with inhomogeneous

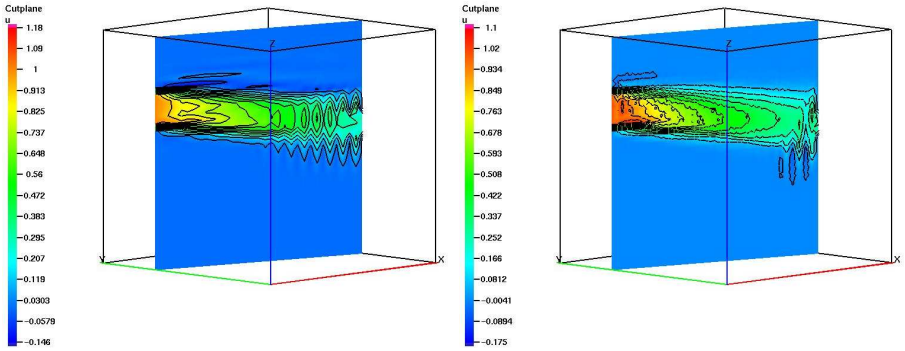

Figure 4: Cut of the solution, SOLD method (4), $C = 0.2$ at $t = 2$, left Q_1, right P_1.

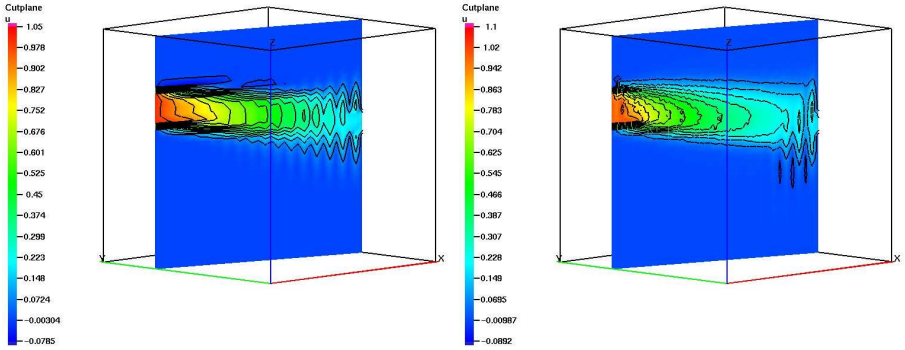

Figure 5: Cut of the solution, SOLD method (4), $C = 0.4$ at $t = 2$, left Q_1, right P_1.

Dirichlet and homogeneous Neumann boundary conditions. The SUPG method led to globally polluted solutions with large spurious oscillations. These oscillations were reduced considerably with a SOLD method, however on the expense of much larger computing times. FEM–FCT methods led to almost oscillation–free solutions. From the aspects of solution quality and computing time, the linear FEM–FCT scheme seems to be, among the studied methods, the most appropriate method to be used in applications.

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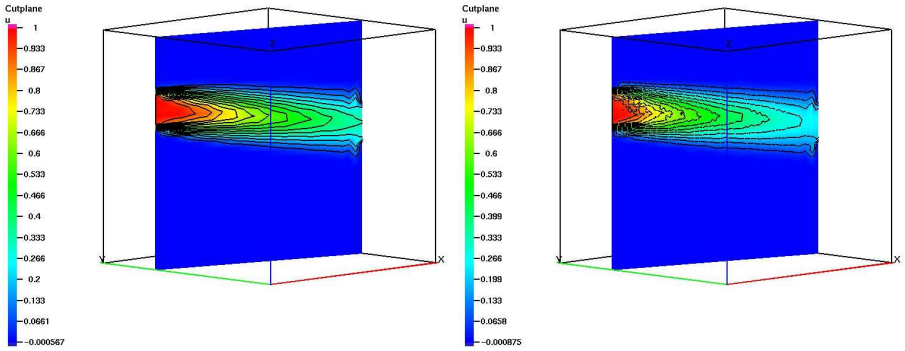

Figure 6: Cut of the solution linear FEM–FCT method at $t = 2$, left Q_1, right P_1.

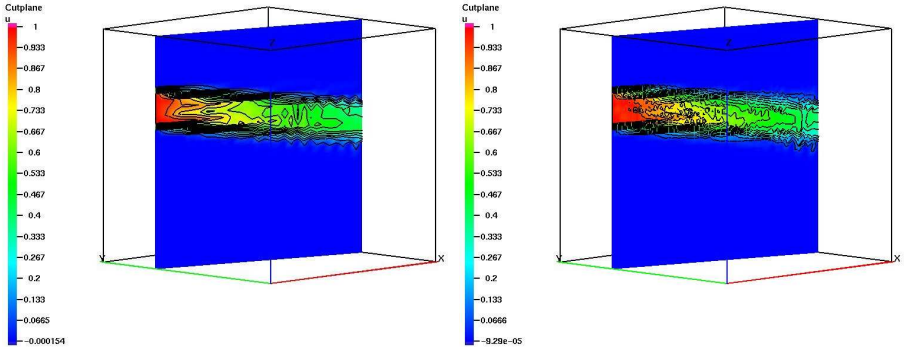

Figure 7: Cut of the solution, nonlinear FEM–FCT method at $t = 2$, left Q_1, right P_1.

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method	Q_1	P_1
SUPG	5989	9473
SOLD (4) $C = 0.2$	24832	25050
SOLD (4) $C = 0.4$	33688	30932
FEM_FCT linear	5920	6509
FEM_FCT nonlinear	9768	10398

Table 1: Computing times in seconds.

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