

Standard and Mixed Finite Elements: A Comparison and Applications in Hydrology

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Abstract

The goal of this paper is to compare the standard and the mixed hybrid finite element methods (FEMs). The relative L_2 errors for pressure and flux are computed with respect to the CPU time which each method needs for solving the corresponding linear algebraic system. Several examples of linear elliptic partial differential equations (PDEs) related to the transport in porous media are presented.

Key words: Standard and mixed hybrid FEM, porous media, error, CPU time

AMS classification: 65N30

1 Introduction

Subsurface contaminant transport is governed by a number of spreading, retardation and transformation mechanisms such as advection, dispersion, diffusion, interfacial mass transfer, adsorption and volatilization, and biological and chemical reactions. It is a multi-phase and multi-component process. Three-dimensional models of movement in a porous medium are based on the macroscopic mass balance equation for component i in phase α (see Abriola and Pinder [1])

$$\partial_t(\rho^\alpha \varepsilon^\alpha \omega_i^\alpha) + \nabla \cdot (\rho^\alpha \mathbf{q}^\alpha \omega_i^\alpha) - \nabla \cdot \mathbf{J}_i^\alpha = \rho^\alpha \varepsilon^\alpha [f_i^\alpha + e_i^\alpha], \quad (1)$$

where $\rho^\alpha \left[\frac{kg}{m^3} \right]$ is the mass density of phase α ; $\varepsilon^\alpha [1]$ is the volume fraction occupied by phase α ; $\mathbf{q}^\alpha \left[\frac{m}{s} \right]$ is the Darcy's velocity of phase α ; $\omega_i^\alpha [1]$ is the mass fraction of component i in phase α ; $\mathbf{J}_i^\alpha \left[\frac{kg}{m^2 s} \right]$ is the flux vector representing the diffusive flux of component i in phase α ; $f_i^\alpha \left[\frac{1}{s} \right]$ is the source of component i in phase α ; $e_i^\alpha \left[\frac{1}{s} \right]$ is the gain of mass of component i due to the phase change.

In fact, the whole situation is much more complicated due to uncertainty of data and corresponding boundary conditions. There exist many numerical methods for solving the subsurface transport. The FEMs are widely used for simulation in applied physics and engineering. These methods are better adapted to general shapes and geometries than the classical finite difference or spectral methods allow.

*The author was supported by the Hanns Seidel Foundation.

¶The author was supported by the BMBF (German Federal Ministry for Education, Science, Research and Technology) Grant Number 03-HO7BWM.

Transport in porous media is in general governed by nonlinear elliptic-parabolic equations. After discretization in time and linearization, each of these equations leads in almost all cases to an elliptic PDE. Thus, in this comparison we consider linear elliptic PDEs which are solved in a domain $\Omega \subset \mathbb{R}^2$. The state variable of the equation is called *pressure* and the *velocity* (which is proportional to the gradient of the pressure) is called *flux*.

The common idea for the FEMs is to triangulate a given domain. In this way one mesh (elements, faces, and vertices) is constructed. The next step is to define appropriate basis functions on each element in order to approximate the pressure and the flux.

We want to compare the two basic approaches, mixed and standard. Both methods use different variational formulations and different functional spaces for the approximation. We consider the simplest conforming standard method, where the pressure is approximated by piecewise linear continuous functions and the flux is obtained by numerical differentiation of the pressure. On the other hand, we consider the mixed hybrid FEM, where the pressure is approximated by piecewise constant functions. For the approximation of the flux the simplest Raviart-Thomas space RT_0 is used. The essential feature of the mixed approach is the continuity of the normal components of the flux on the inter-element boundaries.

For the comparison we have chosen three different problems occurring in subsurface transport. Both approaches (mixed and standard FEM) are compared for these examples taking into account different criteria of errors and efficiency.

All computations were done on a SPARCstation 20 Model 712 with 128 Mb of memory and a 75 MHz processor.

2 A Short Description of Standard and Mixed Finite Elements

In this paper we consider boundary value problems for $u \in H^1(\Omega)$ (called the *pressure field*) of the form

$$\begin{cases} \nabla \cdot \vec{q} = f & \text{in } \Omega \\ \vec{q} = -K \nabla u & \text{in } \Omega \\ u = u_D & \text{on } \Gamma_D \\ q_\nu = q_N & \text{on } \Gamma_N \\ q_\nu \geq 0, u \leq u_S, q_\nu(u - u_S) = 0 & \text{on } \Gamma_S \end{cases}, \quad (2)$$

where Ω is a bounded domain in \mathbb{R}^2 with polygonal boundary $\Gamma = \Gamma_D \cup \Gamma_N \cup \Gamma_S$, the *conductivity* $K \in L_\infty(\Omega)$ a uniformly positive real-valued function on Ω , and the *normal flux* $q_\nu = \vec{q} \cdot \vec{\nu}$ on the boundary (here $\vec{q} = (q_x, q_y)$ is the *flow field* and $\vec{\nu} = (\nu_x, \nu_y)$ the *outer normal* vector on Γ). The distributed data is the *source field* $f \in L_2(\Omega)$, and the boundary data are the *Dirichlet* data $u_D \in H^{1/2}(\Gamma_D)$, the *Neumann* data $q_N \in H^{-1/2}(\Gamma_N)$ and the *Signorini* data $u_S \in H^{1/2}(\Gamma_S)$.

Let us denote a regular triangulation of Ω (cf. Ciarlet [3], Chap. 3) by \mathcal{T}^h with the mesh diameter h . We consider piecewise linear standard finite elements (cf. Ciarlet [3]). Thus, on each element $\mathcal{T} \in \mathcal{T}^h$ we have three linear basis functions associated with the vertices. We compute the approximation u^h and then by postprocessing we obtain \vec{q}^h .

For the mixed hybrid method (see Brezzi and Fortin [2]) we have to approximate simultaneously

- the solution - by piecewise constant functions on \mathcal{T}^h ,
- the flux - by linear functions from the Raviart-Thomas space RT_0 ,
- Lagrange multipliers - by piecewise constant functions on the interior edges of the triangulation \mathcal{T}^h .

This can be done by static condensation, i.e. at first we compute the Lagrange multipliers, then the pressure u^h , and finally the flux \vec{q}^h .

Both numerical methods lead to linear algebraic systems with positive definite matrices, which are solved by the conjugate gradient method (CG) preconditioned by an incomplete Cholesky factorisation.

3 The Methodology of the Comparison

Let (u, \vec{q}) denote the exact solution of the problem (2). The idea of this comparison is to compute a numerical approximation (u^h, \vec{q}^h) , and to evaluate the error of approximation using the following criteria:

1. The relative L_2 error of the pressure given as

$$E_{u,2} = \frac{\sqrt{\int_{\Omega} (u - u^h)^2 dx}}{\sqrt{\int_{\Omega} (u)^2 dx}}.$$

2. The relative L_2 error of the flux

$$E_{q,2} = \frac{\sqrt{\int_{\Omega} (q_x - q_x^h)^2 dx + \int_{\Omega} (q_y - q_y^h)^2 dx}}{\sqrt{\int_{\Omega} (q_x)^2 dx + \int_{\Omega} (q_y)^2 dx}}.$$

3. The relative mass balance error (relative to the total source) defined by

$$E_{mass} = \frac{\int_{\Gamma} q_{\nu}^h d\Gamma - \int_{\Omega} f dx}{\int_{\Omega} f dx}.$$

4. The relative outflow error through the unilateral boundary given as

$$E_{out} = \frac{\int_{\Gamma_S} q_{\nu}^h d\Gamma_S - \int_{\Gamma_S} q_{\nu} d\Gamma_S}{\int_{\Gamma_S} q_{\nu} d\Gamma_S}.$$

All integrals used here are to be understood in the sense of numerical integration. By computations we have tested different quadrature rules but the results were almost the same. Thus, we have chosen for this paper the simplest (midpoint) quadrature rule.

We realize that the best algebraic solver can be different for each numerical method. If one took different solvers for different finite element methods, then the comparison would depend on the computer implementation and thus the results would be misleading. Hence we have taken the same algebraic solver for both standard and mixed FEM.

Let us note that for a given triangulation \mathcal{T}^h each numerical method has a different number of basis functions. Thus it seems not to be reasonable to compare both methods for a fixed mesh. One can expect that the method with a larger number of basis functions will give smaller errors, but the computation will be more time consuming and it will need more memory. Therefore, an appropriate criterion is related to the CPU time needed for computations. On the other hand, for small values of h most of the CPU time is spent (for both numerical methods) for solving the corresponding algebraic system. For these reasons we will show the relation between the CPU time for CG and the corresponding error. In order to make the CG stopping criterion

comparable with the error of discretization we have chosen $\varepsilon_{CG} = Ch^{\frac{4}{3}}$ (the exponent $\frac{4}{3}$ was established empirically). The choice of the constant C for ε_{CG} depends on the example and the method.

It is known that the mixed hybrid and the classical mixed methods are mathematically equivalent (cf. Brezzi and Fortin [2], Chap. V, Th. 1.1). Thus we have $\bar{q}^h \in RT_0(\Omega, \mathcal{T}^h)$. Analyzing the basis functions for the Raviart-Thomas space RT_0 , one can easily see that for an arbitrary edge e between two triangles $\mathcal{T}_1, \mathcal{T}_2 \in \mathcal{T}^h$, the outflow from \mathcal{T}_1 through the edge e is equal to the inflow to \mathcal{T}_2 . That is why the mixed method has an exact mass balance. On the other hand, the standard FEM allows jumps of the normal components of the flux along the interior edges; hence the mass balance cannot be exact. Of course, this is true only if the corresponding algebraic system has been exactly solved, i.e. for $\varepsilon_{CG} = 0$. If $\varepsilon_{CG} > 0$, we cannot compute (u^h, \bar{q}^h) exactly and we will have some small error of the mass balance for the mixed method, which can be diminished by taking sufficiently small ε_{CG} . For this reason we will study the behaviour of the mass balance error with respect to the mesh step h for the standard FEM, only.

The disadvantage of discontinuities of the normal component of the flux on the interelement boundaries for standard FEM can be removed, e.g., by using the method developed by Cordes and Kinzelbach [4]. For the comparison of this modified standard FEM with the mixed FEM we refer the reader to Mose, Siegel, Ackerer and Chavent [9]. We also refer the reader to Cordes and Kinzelbach [5] for the theoretical comparison among finite element, finite volume and finite differences methods.

For all examples considered here the domain Ω is a square in the two-dimensional plane \mathbb{R}^2 . In the following sections we prescribe the conductivity K and the exact solution u in closed form and determine the source f and the boundary data u_D, q_N , and u_S accordingly.

4 Oscillating Coefficients

Analysis of flow in heterogeneous porous media is, in general, very difficult due to spatial variability of the soil. For this reason we have chosen the following example for the comparison between mixed and standard FEMs.

We consider single-phase flow through a highly heterogeneous porous medium. The flow is governed by Darcy's law and can be described by an elliptic PDE with rapidly oscillating coefficients.

Let Ω be a square $[0, L] \times [0, L]$ with $L = \pi$. The boundary is $\Gamma_D = \{(0, y) : 0 < y < L\} \cup \{(L, y) : 0 < y < L\}$, $\Gamma_N = \{(0, y) : 0 < y < L\} \cup \{(L, y) : 0 < y < L\}$, and $\Gamma_S = \emptyset$. The conductivity is oscillatory in space and it is given by

$$K(x, y) = 10^A \sin(Bx) \sin(By).$$

The exact solution chosen is

$$u(x, y) = 1 + \sin(x) \sin(y).$$

We carry out this comparison for two settings of the parameters $(A, B) = (2, 10)$, $(A, B) = (3, 2)$ and for several different uniform meshes. Here the parameter A denotes the amplitude of the soil conductivity and B governs the wave length of the oscillation of the medium. The errors of the pressure $E_{u,2}$ for both settings of parameters are shown in Figure 4.2. Mixed and standard FEMs have the same order of convergence $\mathcal{O}(h^2)$ for the pressure, and the errors are comparable.

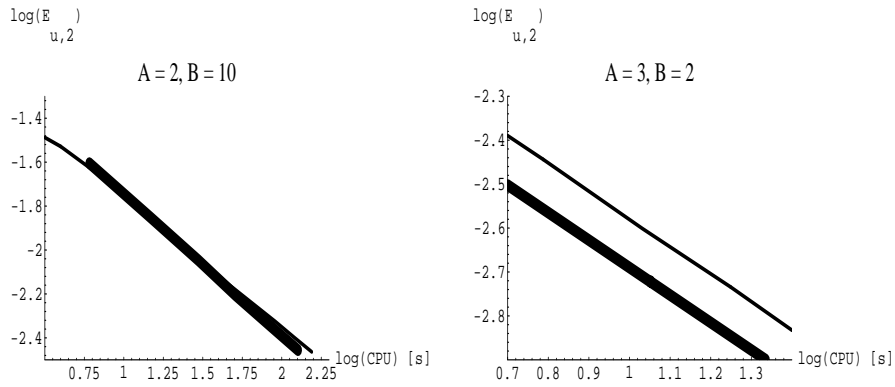


Figure 4.2: Oscillating Coefficients: $E_{u,2}$ (Mixed, Standard)

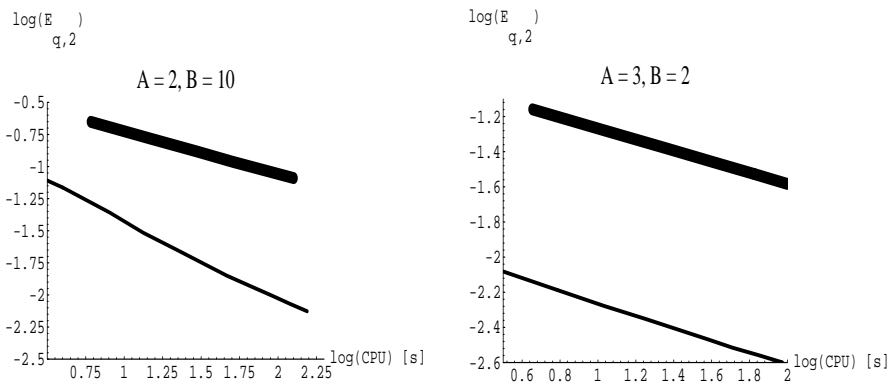


Figure 4.3: Oscillating Coefficients: $E_{q,2}$ (Mixed, Standard)

Flux errors $E_{q,2}$ are drawn in Figure 4.3. Here the order of convergence is $\mathcal{O}(h)$ for both methods and the error is smaller for the standard FEM. The behaviour of the mass balance error E_{mass} for standard element FEM is shown in Figure 4.4.

5 Point Source

Groundwater contamination by nonaqueous phase liquids (NAPL) - due to improper industrial waste disposal and leaking underground storage tanks - has become a serious problem. If the NAPL contaminants are volatile, soil venting, a well established method for soil remediation

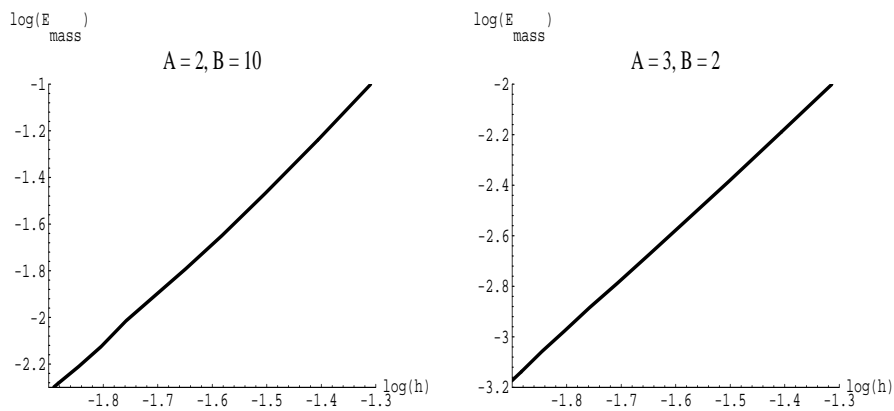


Figure 4.4: Oscillating Coefficients: E_{mass} (Standard FEM)

and cleanup, is often used. The idea is to create an air flow through the contaminated zone and extract the contaminant by a volatilization process. This process involves pumping the gas phase out of the vicinity of the extraction wells. The air flow through the porous medium is governed by Darcy's law, and the active wells can be described as point sinks (see Hornung, Kelanemer and Slodička [8]).

For these reasons we have chosen the following example as our second model problem. We want to solve the problem

$$\left\{ \begin{array}{ll} -\Delta v &= -\frac{2 + \log(x^2 + y^2)}{2\pi} - \delta_0 & \text{in } \Omega \\ v &= \frac{(1 + x^2 + y^2)^\pi \log(x^2 + y^2)}{4\pi} & \text{on } \Gamma_D \\ -\nabla v \cdot \vec{\nu} &= -\frac{1 + \log(x^2 + y^2) + (x^2 + y^2)^{-1}}{2\pi} (x, y) \cdot \vec{\nu} & \text{on } \Gamma_N \end{array} \right. \quad (3)$$

in $\Omega = (-1, 1) \times (-1, 1)$. This problem admits the unique solution given by

$$u(x, y) = a(x, y) \log(x^2 + y^2),$$

where

$$a(x, y) = \frac{1 + x^2 + y^2}{4\pi}.$$

Let us transform (3) into

$$\left\{ \begin{array}{ll} -\Delta \tilde{v} &= -\frac{2 + \log(x^2 + y^2)}{2\pi} & \text{in } \Omega \\ \tilde{v} &= \frac{(x^2 + y^2)^\pi \log(x^2 + y^2)}{4\pi} & \text{on } \Gamma_D \\ -\nabla \tilde{v} \cdot \vec{\nu} &= -\frac{1 + \log(x^2 + y^2)}{2\pi} (x, y) \cdot \vec{\nu} & \text{on } \Gamma_N. \end{array} \right. \quad (4)$$

This has the unique solution defined as

$$\tilde{u}(x, y) = u(x, y) - u_0(x, y),$$

where

$$u_0(x, y) = a(0, 0) \log(x^2 + y^2) = \frac{\log(x^2 + y^2)}{4\pi}.$$

This idea of subtracting the singular part from the solution can be found in the literature, e.g., Douglas, Ewing and Wheeler [6]. The errors $E_{u,2}$ and $E_{q,2}$ are drawn in Figure 5.5. The orders for both numerical methods are the same as for the oscillatory coefficients, but now the errors are smaller for the mixed method. The mass balance error E_{mass} for standard element FEM is shown in Figure 5.6.

6 Unilateral Boundary Conditions

When a landfill is exposed to rainfall, the infiltrating water may become contaminated. To prevent this, one can construct a capillary barrier. In principle, this consists of a two-layered system of granular material with a sloping interface (bottom coarse and top fine layer). Due to the capillary forces recharging water will be stored in the fine layer and drain off laterally rather than infiltrate downwards. The effectivity of such a system can be measured by the lateral

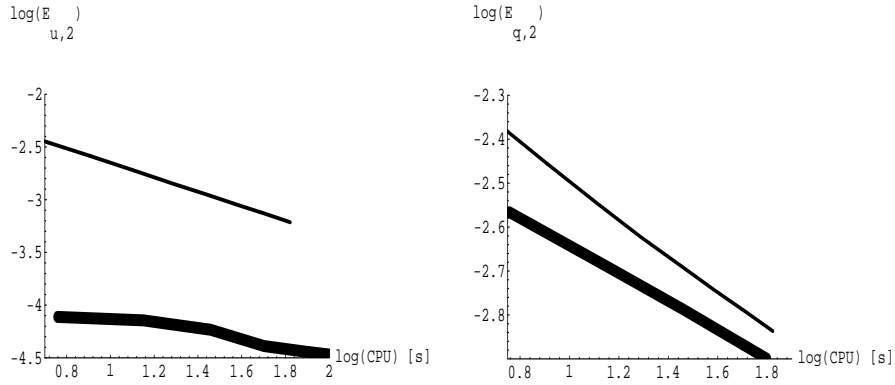


Figure 5.5: Point Source: $E_{u,2}, E_{q,2}$ (Mixed, Standard)

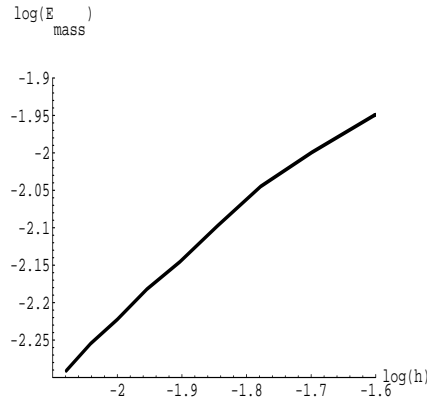


Figure 5.6: Point Source: E_{mass} (Standard FEM)

outflow in the layers relative to the amount of infiltrated precipitation. The water will flow out through the boundaries during saturation.

One possibility how to mathematically model this kind of boundary conditions is to use the ‘Signorini-problem’ (unilateral boundary conditions UBC, cf. Glowinski, Lions and Trémolières [7]). That means that the situation on the boundary will change as follows: the flux is zero when unsaturated conditions are achieved, otherwise, the outward component of the flux is positive.

In the following example we solve a Poisson equation (the conductivity $K = 1$) in the domain $\Omega = [0, L] \times [0, L]$ ($L = 1$) with the right-hand side f and the boundary data u_D and g_N , according to the exact solution given in closed form

$$u(x, y) = -A(Y_0 - y)_+^3 - B(y - Y_0)_+^3(x - L) + C(x - L)^2 \sin(y - Y_0)_+^3,$$

where A, B, C, L and Y_0 are real parameters and the function $(\cdot)_+$ is the truncation function: $(y)_+ = \max\{y, 0\}$.

The boundaries are $\Gamma_D = \{(0, y) : 0 \leq y \leq L\}$, $\Gamma_N = \{(x, 0) : 0 < x < L\} \cup \{(x, L) : 0 < x < L\}$, $\Gamma_S = \{(L, y) : 0 \leq y \leq L\}$ and $u_S = 0$.

When the parameters A and B are positive and $0 < Y_0 < L$, we can observe that u satisfies the Signorini conditions on one part of the boundary $x = L$, roughly speaking, $u \leq 0$ and $q_\nu = 0$ on $\{(L, y) : 0 \leq y \leq Y_0\}$ and $u = 0$ and $q_\nu > 0$ on $\{(L, y) : Y_0 < y \leq L\}$. We let the parameters take the values $A = 1$, $B = 1$, $C = 3$, and $Y_0 = 0.5$. We solve this problem by an iterative process until the solution satisfies the unilateral condition on Γ_S . The problem has numerically been solved with both (standard and mixed hybrid) FEMs. The results show that the global relative L_2 errors $E_{u,2}$ for the pressure (Figure 6.7) and the flux $E_{q,2}$ (Figure 6.8), for the same

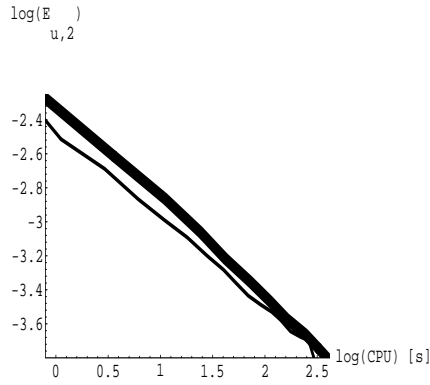


Figure 6.7: UBC: $E_{u,2}$ (**Mixed**, Standard)

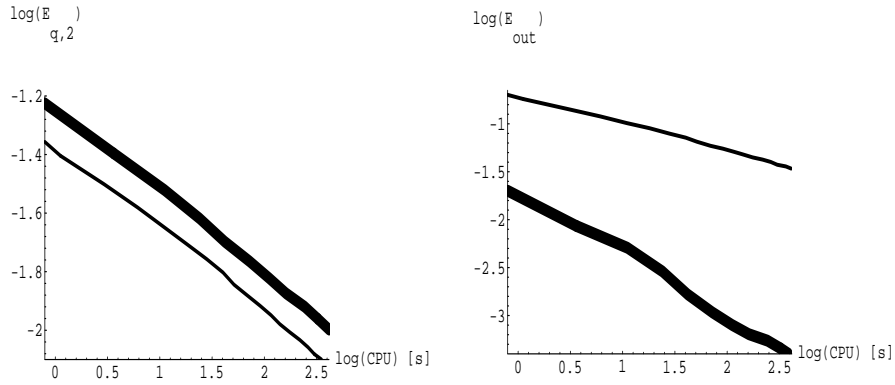


Figure 6.8: UBC: $E_{q,2}$, E_{out} (**Mixed**, Standard)

CPU time, are a little less for standard FEM. On the other hand, the outflow error E_{out} on the Γ_S is 10 times larger for the standard method than for the mixed method (Figure 6.8). The behaviour of the absolute outflow error on the unilateral boundary Γ_S ($x = 1$) is drawn in Figures 6.9, 6.10 for different CPU times. Here the mixed hybrid FEM is superior to the standard method.

7 Conclusions

- The mixed FEM has an exact mass balance (this follows from the definition of the RT_0 space). The standard FEM does not have this property, but the relative mass balance error can be made small enough for sufficiently small h (see Figures 4.4, 5.6).
- A consequence of the mass preservation of mixed FEM are better results for the flux through the boundary E_{out} , but the order of convergence for both methods seems to be the same (Figure 6.8).
- The situation with $E_{u,2}$ and $E_{q,2}$ is more complicated. For the point source example the mixed hybrid method is better; on the other hand for unilateral boundary conditions (UBC) the opposite is true. For the example with oscillating coefficients $E_{u,2}$ is almost the same for both methods and $E_{q,2}$ is much better for standard FEM. Both numerical methods have the same order of convergence $\mathcal{O}(h^2)$ for $E_{u,2}$ and $\mathcal{O}(h)$ for $E_{q,2}$ (taking into account the superconvergence properties). The exact mass balance for

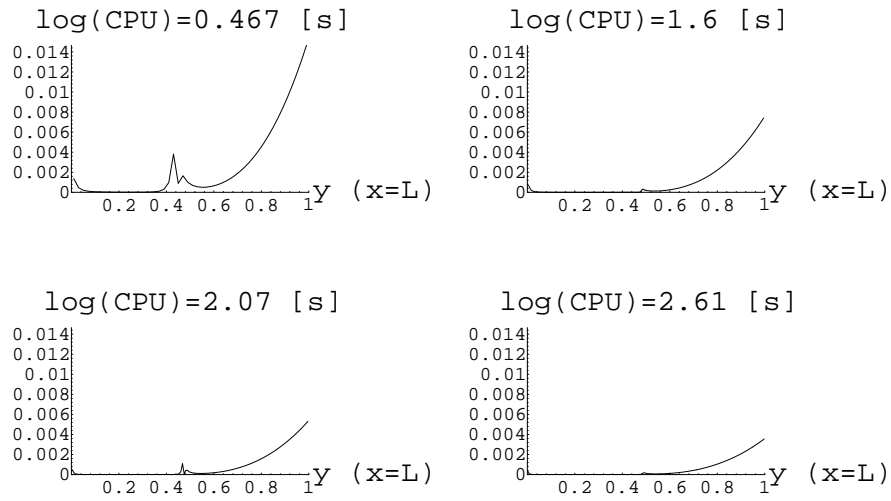


Figure 6.9: UBC: The outflow error on Γ_S (Standard FEM)

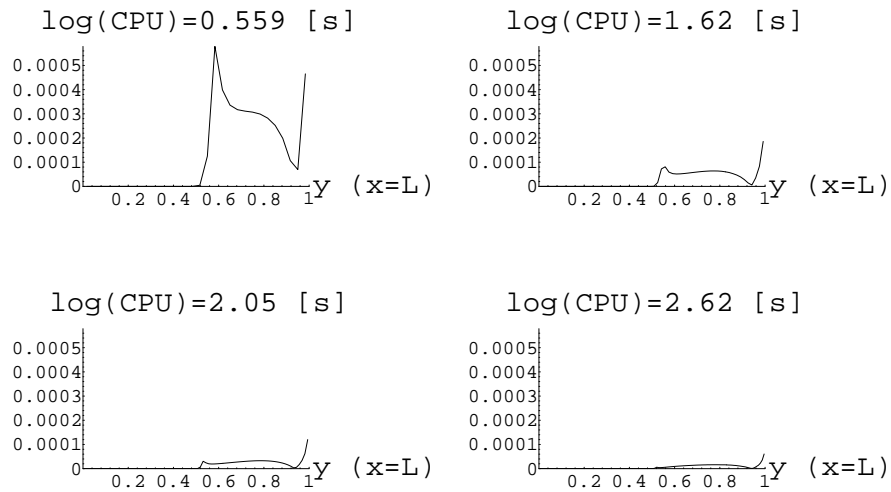


Figure 6.10: UBC: The outflow error on Γ_S (Mixed FEM)

mixed FEM does not imply the fact that the $E_{q,2}$ error will be smaller for mixed than for standard FEM.

The examples studied show that before deciding on the choice of a numerical algorithm, one should carefully investigate the following aspects:

- the type of problem which has to be solved,
- the most important error criterion for the solution (potential, flux, outflow, ...),
- hardware restrictions (memory, speed of computations, ...).

The standard FEM may be superior in one situation, whereas mixed FEM may be better in another.

Remark Here we have made comparisons for linear elliptic differential equations. We realize that for nonlinear or time dependent problems new aspects can arise that may lead to results different from the conclusions presented here.

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