A Decoupled Iterative Method for Mixed Problems using Divergence-free Finite Elements*

(Extended Abstract)

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Introduction

The problem we are going to consider in this paper is the following second-order elliptic problem in velocity-pressure formulation

$$\vec{u} + K\,\vec{\nabla} p \;=\; \vec{g}\;, \tag{1}$$
$$\vec{\nabla}\cdot\vec{u} \;=\; 0\;, \tag{2}$$

over a polyhedral simply connected three-dimensional domain Ω. Such a problem arises for example in groundwater flow or oil recovery simulations, where $\vec{u}$ corresponds to the velocity, p to the pressure, and K is permeability divided by dynamic viscosity. We are interested in solving system (1), (2) subject to mixed boundary conditions

$$p = p_D \quad \text{on} \quad \Gamma_D, \qquad \text{and} \quad \vec{u}\cdot\vec{\nu} = 0 \quad \text{on} \quad \Gamma_N\;, \tag{3}$$

where Γ_D and Γ_N are assumed to partition the boundary of Ω, and $\vec{\nu}(\vec{x})$ denotes the outward unit normal from Ω at $\vec{x} \in \Gamma_N$. Additionally we assume that each connected component of Γ_N is simply connected.

The numerical treatment of (1 - 3) involves the solution of usually very large indefinite linear equation systems. In this paper we describe a very efficient and practicable iterative method to solve these systems by decoupling the vector of velocities from the vector of pressures, resulting in a symmetric positive definite velocity system and a triangular pressure system. The crucial step in this approach is the construction of a basis for the divergence-free Raviart-Thomas-Nédélec elements (using results from Algebraic Topology and Graph Theory).

Mixed Finite Element Discretisation

We discretise (1 - 3) using the lowest order mixed Raviart-Thomas-Nédélec elements on tetrahedral meshes ([8]). First we put (1 - 3) in weak form. We introduce the space

$$H_{0,N}(\mathrm{div},\Omega) := \{\vec{v} \in L_2(\Omega)^3 : \mathrm{div}\,\vec{v} \in L_2(\Omega) \text{ and } \vec{v}\cdot\vec{\nu}|_{\Gamma_N} = 0\},$$

Then the weak form of (1 - 3) is to find $(\vec{u}, p) \in H_{0,N}(\mathrm{div},\Omega) \times L_2(\Omega)$ such that

$$\left.\begin{array}{rcl} (K^{-1}\vec{u},\vec{v})_{L_2} - (\mathrm{div}\,\vec{v}, w)_{L_2} &=& G(\vec{v})\;, \quad \text{for all } \vec{v} \in H_{0,N}(\mathrm{div},\Omega), \\ -(\mathrm{div}\,\vec{v}, w)_{L_2} &=& 0\;, \quad \text{for all } w \in L_2(\Omega). \end{array}\right\} \tag{4}$$

with $G(\vec{v}) := (K^{-1}\vec{g},\vec{v})_{L_2} - \int_{\Gamma_D} p_D\,\vec{v}\cdot d\vec{\nu}$.

To discretise (4) by Raviart-Thomas-Nédélec elements we introduce a triangulation $\mathcal{T}$ of Ω into conforming tetrahedra $T \in \mathcal{T}$, and approximate $\vec{u}$ and p in finite dimensional subspaces of $H_{0,N}(\mathrm{div},\Omega)$ and $L_2(\Omega)$. Here p is approximated in the space $\mathcal{W}$ of piecewise constant functions with basis consisting of the characteristic functions w_T of each of the tetrahedra $T \in \mathcal{T}$, and $\vec{u}$ is approximated in an appropriate subspace $\mathcal{V}$ of the vector-valued piecewise linear functions in which the normal component of $\vec{u}$ is required to be continuous across the element boundaries.

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Let $\mathcal{F}$ denote the set of all faces of the tetrahedra in $\mathcal{T}$ which is assumed partitioned into $\mathcal{F}_I \cup \mathcal{F}_D \cup \mathcal{F}_N$ of faces $F \in \mathcal{F}$ which lie in Ω, Γ_D and Γ_N, respectively. For any $F \in \mathcal{F}$, let $\vec{\nu}_F$ denote the unit normal to the face F (with orientation fixed). Then we define the basis of $\mathcal{V}$ by associating with each face $F \in \mathcal{F}_I \cup \mathcal{F}_D$ a vector-valued piecewise linear function $\vec{v}_F \in \mathcal{V}$ of the form $\vec{v}_F(\vec{x}) = \vec{\alpha}_T + \gamma_T \vec{x}$ on each $T \in \mathcal{T}$, with the property that $\vec{v}_F \cdot \vec{\nu}_{F'} = \delta_{F,F'}$ for all $F' \in \mathcal{F}_I \cup \mathcal{F}_D$. The resulting discretisation enforces mass conservation on each element of the mesh, and the resulting linear equations system is of saddle-point form:

$$\begin{pmatrix} M & B \\ B^T & 0 \end{pmatrix} \begin{pmatrix} \mathbf{u} \\ \boldsymbol{p} \end{pmatrix} = \begin{pmatrix} \mathbf{g} \\ \mathbf{0} \end{pmatrix} \quad \text{in} \quad \mathbb{R}^{n_{\mathcal{V}}} \times \mathbb{R}^{n_{\mathcal{W}}} , \tag{5}$$

where $M_{F,F'} := (K^{-1}\vec{v}_F, \vec{v}_{F'})_{L_2}$, $B_{F,T} := -(\operatorname{div} \vec{v}_F, w_T)_{L_2}$, $g_F := G(\vec{v}_F)$, and the dimensions are $n_{\mathcal{V}} = (\#\mathcal{F}_I + \#\mathcal{F}_D)$ and $n_{\mathcal{W}} = (\#\mathcal{T})$.

Decoupled Iterative Method for Mixed Problems

In this section we formulate our method for decoupling the vector of velocities $\boldsymbol{u}$ from the vector of pressures $\boldsymbol{p}$ in system (5). This procedure has already been presented for the 2D case in [3]. Recall ([1]) that (5) has a unique solution $(\boldsymbol{u}, \boldsymbol{p}) \in \mathbb{R}^{n_{\mathcal{V}}} \times \mathbb{R}^{n_{\mathcal{W}}}$ for all $\mathbf{g} \in \mathbb{R}^{n_{\mathcal{V}}}$, and clearly $\boldsymbol{u}$ is in $\ker B^T$.

The decoupling of $\boldsymbol{u}$ from $\boldsymbol{p}$ can be achieved by finding a basis $\{\mathbf{z}_1, \ldots, \mathbf{z}_{\mathring{n}}\}$ of $\ker B^T$. (Since B^T has full rank, $\mathring{n} = n_{\mathcal{V}} - n_{\mathcal{W}}$.) If we have such a basis, then the solution $\boldsymbol{u}$ of (5) can be written

$$\boldsymbol{u} = \sum_{j=1}^{\mathring{n}} \mathring{u}_j \mathbf{z}_j = Z^T \mathring{\boldsymbol{u}} ,$$

for some $\mathring{\boldsymbol{u}} \in \mathbb{R}^{\mathring{n}}$, where Z denotes the $\mathring{n} \times n_{\mathcal{V}}$ matrix with rows $\mathbf{z}_1^T, \ldots, \mathbf{z}_{\mathring{n}}^T$. Also, since $ZB = (B^T Z^T)^T = 0$, multiplying the first (block) row of (5) by Z shows that $\mathring{\boldsymbol{u}}$ is a solution of the linear system

$$\mathring{A}\mathring{\boldsymbol{u}} = \mathring{\mathbf{g}} \tag{6}$$

where $\mathring{A} = ZMZ^T$ and $\mathring{\mathbf{g}} = Z\mathbf{g}$. Since M is symmetric positive definite, so is $\mathring{A}$ and $\mathring{\boldsymbol{u}}$ is the unique solution of (6). Thus if the basis $\{\mathbf{z}_1, \ldots, \mathbf{z}_{\mathring{n}}\}$ can be found then the velocity $\boldsymbol{u}$ in (5) can be computed by solving the decoupled positive definite system (6) rather than the indefinite coupled system (5). Moreover the system (6) is about 3 times smaller than (5).

In applications to groundwater flow, where one is primarily interested in the velocity $\vec{u}$ in (1), (2), the method described above is of great relevance. Even when the pressure p is also of interest our method may still be highly competitive, provided we can also compute a *complementary basis* $\{\mathbf{z}_{\mathring{n}+1}, \ldots, \mathbf{z}_{n_{\mathcal{V}}}\}$ with the property that $\operatorname{span}\{\mathbf{z}_1, \ldots, \mathbf{z}_{\mathring{n}}, \mathbf{z}_{\mathring{n}+1}, \ldots, \mathbf{z}_{n_{\mathcal{V}}}\} = \mathbb{R}^{n_{\mathcal{V}}}$. If this is known and if Z' denotes the matrix with rows $\mathbf{z}_{\mathring{n}+1}^T, \ldots, \mathbf{z}_{n_{\mathcal{V}}}^T$, then multiplying the first (block) row of (5) by Z' shows that $\boldsymbol{p}$ is the solution of the $n_{\mathcal{W}} \times n_{\mathcal{W}}$ system

$$(Z'B)\boldsymbol{p} = Z'(\mathbf{g} - M\boldsymbol{u}) . \tag{7}$$

An elementary argument shows that $Z'B$ is non-singular and so the unique solution $\boldsymbol{p}$ of (7) also determines the pressure in (5) once the velocity $\boldsymbol{u}$ is known. Exploiting the particular form of (5), a simple choice of complementary basis can be made so that $Z'B$ is triangular (see below).

Construction of a Divergence-free Basis

Note that finding the basis $\mathbf{z}_1, \ldots, \mathbf{z}_{\mathring{n}}$ in the previous section is equivalent to finding a basis $\vec{\mathring{v}}_1, \ldots, \vec{\mathring{v}}_{\mathring{n}}$ of the space $\mathring{\mathcal{V}} := \{\vec{V} \in \mathcal{V} : b(\vec{V}, W) = 0 \text{ for all } W \in \mathcal{W}\}$ of divergence-free Raviart-Thomas-Nédélec elements. We construct this basis from the curls of Nédélec's edge elements ([8]).

First of all, let $\mathcal{E}$ denote the set of all edges of the tetrahedra in $\mathcal{T}$ which is assumed partitioned into $\mathcal{E}_I \cup \mathcal{E}_D \cup \mathcal{E}_N$ of edges $E \in \mathcal{E}$ which lie in Ω, Γ_D and Γ_N, respectively. For any $E \in \mathcal{E}$, let $\vec{\tau}_E$ denote the unit tangent on edge E (with orientation fixed). Now we can introduce the space $\mathcal{U} \subset H(\vec{\operatorname{curl}}, \Omega) := \{\vec{\Phi} \in L_2(\Omega)^3 : \vec{\operatorname{curl}}\, \vec{\Phi} \in L_2(\Omega)^3\}$ of vector-valued piecewise linear functions of the form $\vec{\Phi}(\vec{x}) = \vec{\alpha}_T + \vec{\beta}_T \times \vec{x}$ on each tetrahedron $T \in \mathcal{T}$, in which the tangential component of $\vec{\Phi}$ is required to be continuous along each edge E of the triangulation. We define a basis of $\mathcal{U}$ by associating with each edge $E \in \mathcal{E}$ a function $\vec{\Phi}_E \in \mathcal{U}$ with the property that $\int_{E'} \vec{\Phi}_E \cdot \vec{\tau}_{E'} = \delta_{E,E'}$ for all $E' \in \mathcal{E}$. This choice of basis functions accounts for the widely used term *edge elements*.

The basis for $\mathring{\mathcal{V}}$ will now be constructed from the fundamental functions $\vec{\Psi}_E$ defined by:

$$\vec{\Psi}_E = \vec{\operatorname{curl}}\vec{\Phi}_E, \qquad E \in \mathcal{E}$$

(so that $\vec{\Phi}_E$ is the *vector potential* of $\vec{\Psi}_E$). The following theorem identifies a linearly independent subset of the functions $\vec{\Psi}_E$, $E \in \mathcal{E}$, that constitutes a basis of $\mathring{\mathcal{V}}$. The proof involves some fundamental notions and results from Graph Theory and Algebraic Topology. In particular we need the notion of *spanning tree* of a graph.

Let $\mathbf{G} := (\mathcal{N}, \mathcal{E})$ be the graph formed by the nodes $\mathcal{N}$ and (orientated) edges $\mathcal{E}$ of the triangulation $\mathcal{T}$. Furthermore, let $n_{\mathcal{C}}$ denote the number of connected components in Γ_N, and write $\Gamma_N = \Gamma_N^1 \cup \Gamma_N^2 \cup \ldots \cup \Gamma_N^{n_\mathcal{C}}$, where $\Gamma_N^\ell \cap \Gamma_N^{\ell'} = \emptyset$ for all $\ell \neq \ell' \in \{1, \ldots, n_{\mathcal{C}}\}$.

Theorem 1 *Let $\mathcal{H} \subset \mathcal{E}$ be such that $\mathbf{H} := (\mathcal{N}, \mathcal{H})$ is a spanning tree of $\mathbf{G}$, and such that for each $\ell = 1, \ldots, n_{\mathcal{C}}$, the restriction of $\mathbf{H}$ to nodes and edges on Γ_N^ℓ, is also a tree. Then*

$$\{\vec{\Psi}_E : E \in (\mathcal{E}_I \cup \mathcal{E}_D)\backslash\mathcal{H}\} \quad \textit{is a basis of} \quad \mathring{\mathcal{V}}.$$

A similar statement for the pure Neumann case, $\Gamma_D = \emptyset$, has already been proved by Dubois [4], where he uses it to solve model incompressible flow problems with prescribed vorticity. Our proof of Theorem 1 makes use of the methods of Hecht [5] developed for the non-conforming P1-P0 elements for the approximation of divergence-free vector fields in $H^1(\Omega)^3$. In an unpublished manuscript [6], Hecht extends these results to a wider family of finite elements including the Raviart-Thomas-Nédélec elements. In the context of (1), (2) the only other work which we are aware of is the recent paper [2], but this is restricted to uniform rectangular meshes and a special spanning tree which can be constructed a priori.

Implementation

To implement the decoupled system (6) for determining $\mathring{\boldsymbol{u}}$ (and hence $\boldsymbol{u}$) we must work with the matrix $\mathring{A} = ZMZ^T$ and right hand side $\mathring{\mathbf{g}} = Z\mathbf{g}$. We observe that these are formally defined in terms of multiplications with the matrix Z which represents the basis $\{\vec{\Psi}_E : E \in (\mathcal{E}_I \cup \mathcal{E}_D)\backslash\mathcal{H}\}$ of $\mathring{\mathcal{V}}$ in terms of the basis $\{\vec{v}_F : F \in \mathcal{F}_I \cup \mathcal{F}_D\}$ of $\mathcal{V}$. Thus we can identify the columns of Z with the indices $F \in \mathcal{F}_I \cup \mathcal{F}_D$, whereas the rows of Z correspond to $E \in (\mathcal{E}_I \cup \mathcal{E}_D)\backslash\mathcal{H}$, and write

$$\vec{\Psi}_E = \sum\nolimits_{F \in \mathcal{F}_I \cup \mathcal{F}_D} Z_{E,F}\, \vec{v}_F, \qquad E \in (\mathcal{E}_I \cup \mathcal{E}_D)\backslash\mathcal{H}\,.$$

Note that the matrix Z is sparse, in fact $Z_{E,F} \neq 0$ only when E is an edge of F. Therefore it is simple to see that $\mathring{A}$ can be written as a sum of element matrices and $\mathring{\mathbf{g}}$ can be written as a sum of element vectors. This representation may be important if iterative methods are used to solve (6). Also, the set $\mathcal{H} \subset \mathcal{E}$ of edges that form a spanning tree in the graph $\mathbf{G} = (\mathcal{N}, \mathcal{E})$ can be found in optimal time (proportional to the number of edges).

Alternatively $\mathring{A}$ can be determined from an approximation of the related bilinear form

$$a(\vec{\Phi}, \vec{\Phi}') := (K^{-1}\, \vec{\operatorname{curl}}\vec{\Phi}, \vec{\operatorname{curl}}\vec{\Phi}')_{L^2(\Omega)^3} \qquad \text{for all } \vec{\Phi}, \vec{\Phi}' \in H(\vec{\operatorname{curl}}, \Omega)\,,$$

by Nédélec's edge-elements $\vec{\Phi}_E$, without the assembly of any Raviart-Thomas stiffness matrix entries:

Theorem 2

$$\mathring{A}_{E,E'} = a(\vec{\Phi}_E, \vec{\Phi}_{E'}) \qquad \textit{for all } E, E' \in (\mathcal{E}_I \cup \mathcal{E}_D)\backslash\mathcal{H}.$$

We would like to note here that in [7] a multilevel preconditioned conjugate gradient method is presented for solving the singular, symmetric positive semidefinite system with stiffness matrix $\mathcal{A} := (a(\vec{\Phi}_E, \vec{\Phi}_{E'}))_{E,E' \in \mathcal{E}}$ without explicitly eliminating columns and rows corresponding to edges $E \in \mathcal{H}$. In their multilevel splitting they eliminate the kernel of $a(\cdot,\cdot)$ only approximately by relaxing the orthogonality condition and thus avoid the construction of a basis. Here we eliminate the kernel *a priori*.

Pressure computations

The assembly of (7) requires the computation of a complementary basis $\{\mathbf{z}_{\mathring{n}+1}, \ldots, \mathbf{z}_{n_\mathcal{V}}\}$ to $\{\mathbf{z}_1, \ldots, \mathbf{z}_{\mathring{n}}\}$. This is again equivalent to finding a complementary basis $\{\vec{v}^c_{\mathring{n}+1}, \ldots, \vec{v}^c_{n_\mathcal{V}}\}$ to the basis $\{\mathring{\vec{v}}_1, \ldots, \mathring{\vec{v}}_{\mathring{n}}\}$ of $\mathring{\mathcal{V}}$ in $\mathcal{V}$ such that $\mathrm{span}\{\mathring{\vec{v}}_1, \ldots, \mathring{\vec{v}}_{\mathring{n}}, \vec{v}^c_{\mathring{n}+1}, \ldots, \vec{v}^c_{n_\mathcal{V}}\} = \mathcal{V}$.

In the context of the specific system (5) this can be done by finding a distinguished subset of faces

$$\mathcal{F}^c \subset \mathcal{F}_I \cup \mathcal{F}_D$$

such that the corresponding subset $\{\vec{v}_F : F \in \mathcal{F}^c\}$ of Raviart-Thomas-Nédélec basis functions constitutes a complementary basis. Note that this set must contain $n_\mathcal{W} := n_\mathcal{V} - \mathring{n} = \#\mathcal{T}$ elements. The following simple algorithm chooses $n_\mathcal{W}$ appropriate faces:

1. Choose $T_1 \in \mathcal{T}$ to be any tetrahedron with a face $F_1 \in \mathcal{F}_D$ and set $\mathcal{F}^c = \{F_1\}$.
2. For $j = 2, \ldots, n_\mathcal{W}$,
   - choose $T_j \in \mathcal{T} \backslash \{T_\ell : \ell = 1, \ldots, j-1\}$ and $F_j \subset \overline{T}_j$ with the property that there exists $\ell \in \{1, \ldots, j-1\}$ such that
   $$F_j \subset \overline{T}_\ell$$
   - update $\mathcal{F}^c = \mathcal{F}^c \cup \{F_j\}$.
3. Assemble $Z'B$ as $(Z'B)_{i,j} = b(\vec{v}_{F_i}, w_{T_j})$, for all $i, j = 1, \ldots, n_\mathcal{W}$.

Theorem 3 *The above algorithm works, the functions*

$$\{\vec{v}_F : F \in \mathcal{F}^c\}$$

form a complementary basis to $\{\vec{\Psi}_E : E \in (\mathcal{E}_I \cup \mathcal{E}_D) \backslash \mathcal{H}\}$ *in* $\mathcal{V}$ *and the matrix* $Z'B$ *given in Step 3 is lower triangular.*

Using this complementary basis and applying the general theory presented above, we can therefore find the unique solution $\mathbf{p}$ from (7) by simple *back substitutions*.

Numerical Results

We tested the performance of the proposed method for (1 - 3) on two simple problems. Let $\Omega = (0,1)^3$, $K \equiv 1$, $\vec{g} = \vec{0}$ and $p_D = 1 - x$. The two problems are induced by different partitionings of the boundary. In the *first problem* we choose $\Gamma_D = \{0,1\}\times(0,1)\times(0,1) \cup [0,1]\times(0,1)\times\{1\}$, in the *second problem* we choose $\Gamma_D = (0,1)\times(0,1)\times\{1\}$ (in both cases $\Gamma_N = \partial\Omega\backslash\Gamma_D$).

We discretise these problems on a sequence of uniform and non-uniform tetrahedral meshes of different refinement levels L. To solve the resulting saddle-point system (5) we use the decoupled iterative method described above. The subtask of solving the symmetric positive definite system (6) is carried out by ILU-preconditioned conjugate gradients (PCG) until achieving a relative reduction of the residual by a factor of 10^{-5}.

Our results show (as expected) that the work needed for the decoupling process and the recovery of the pressure is proportional to the number of freedoms in (5), and therefore optimal. The core part of the calculation is the solution of (6), and PCG performs as predicted for a 2nd-order elliptic problem. The growth in the number of iterations on the uniform meshes is proportional to $\mathring{n}^{1/3}$ where $\mathring{n}$ is the number of freedoms. We then compared the performance of our method with the performance of a preconditioned *minimum residual* method (MINRES) for the (full mixed) saddle-point system (5) (again the convergence criterion is the relative reduction of the residual by a factor of 10^{-5}). To precondition MINRES we take the ILU factorisation of an optimal block preconditioner presented and analysed in [9]. The results for the second problem are presented in Table 1. Comparing Columns 6 and 7 in Table 1 we observe that

	# Freedoms		Iterations		MFlops	
Mesh	Mixed	Decoupled	Mixed	Decoupled	Mixed	Decoupled
Uniform ($L=4$)	1088	320	62	18	4.2	0.62
8	8960	2816	113	35	66	8.7
16	72704	23552	217	75	1040	132
Non-un. ($L=2$)	544	160	113	24	3.8	0.35
4	4480	1408	255	80	74	8.0
8	36352	11776	460	187	1400	145

Table 1: Comparison of the decoupled iterative method with MINRES (2nd problem)

our decoupled method is almost 8 times faster than preconditioned MINRES on the uniform meshes (Rows 3 – 5), and almost 10 times faster on the non-uniform meshes (Rows 6 – 8).

REFERENCES

[1] F. Brezzi and M. Fortin, *Mixed and Hybrid Finite Element Methods* (Springer, New York, 1991).

[2] Z. Cai, R.R. Parashkevov, T.F. Russell, and X. Ye, Domain decomposition for a mixed finite element method in three dimensions, to appear in *SIAM J Num. Anal.* (1998).

[3] K.A. Cliffe, I.G. Graham, R. Scheichl, L. Stals, Parallel computation of flow in heterogeneous media modelled by mixed finite elements, Bath Math. Prepr. 99/16 (submitted to *J Comp Physics*, 1999).

[4] F. Dubois, Discrete vector potential representation of a divergence-free vector field in three-dimensional domains: Numerical analysis of a model problem, *SIAM J Num. Anal.* **27**, 5 (1990).

[5] F. Hecht, Construction d'une base de fonctions P1 non-conformes à divergence nulle dans $\mathbb{R}^3$, *RAIRO Model. Math. et Anal. Num.* **15** (1981).

[6] F. Hecht, Construction d'une base pour des éléments finis mixtes à divergence faiblement nulle, Unpublished report (1988).

[7] R. Hiptmair and R.H.W. Hoppe, Multilevel methods for mixed finite elements in three dimensions, *Numer. Math.* **82**, 2 (1999).

[8] J.C. Nédélec, Mixed finite elements in $\mathbb{R}^3$, *Numer. Math.* **35** (1980).

[9] T. Rusten and R. Winther, A preconditioned iterative method for saddlepoint problems, *SIAM J. Matrix Anal. Appl.* **13**, 3 (1992).