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SOLVING 3D DIFFUSION EQUATIONS USING NONCONFORMING FINITE ELEMENTS

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Abstract. Nonconforming finite element spaces associated with a fine grid generated by multilevel refinement for solving diffusion equations using simple rotated multilinear basis functions is considered. The existence of hierarchy of grids is exploited to generate coarse–grid spaces in an algebraic manner so that the resulting coarse–grid problems are as sparse as the original matrix. A new multilevel method based on algebraic generation of the coarse finite element space and respective stiffness matrices and by the matrix generated interpolation and restriction procedures is used as a preconditioner in the preconditioned conjugate gradient (PCG) iterative method to solve the resulting symmetric system of linear algebraic equations. The good performance of the method is illustrated with numerical results on a two–dimensional model test problem.

1. Introduction

Multigrid methods for nonconforming finite elements have been studied by many authors (see e.g. [3], [5], [6], [8], [9] [10]). A core in the construction of multilevel cycle is the way one generates the coarse–grid spaces and respective discretization problems and the mappings for intergrid data transformations. A suitable way turns out to be an algebraic generation of the coarse–grid operators by a sort of incomplete factorization procedure working on element by element basis. In Reusken [8] one first gets a two–level block structure of the matrix, with one of the major blocks corresponding to the coarse–grid nodes and the first block on the diagonal corresponding to the complementary node set. By eliminating in a ILU–fashion the block corresponding to the complementary node set one ends up with a matrix, that is considered as a coarse–grid discretization of the original problem. An essential feature here is to keep a prescribed sparsity pattern of the thus obtained coarse–grid matrix in order to be able to recursively apply the same procedure on the currently available discretization matrix. One also constructs in this way (by the ILU–type elimination) matrix dependent intergrid date transfer operators giving rise to restriction and interpolation operators in multigrid methods (MG).

In this report we have chosen nonconforming finite element discretization of diffusion problems for two reasons. First, the nonconforming elements are well suited for more complicated problems like elasticity and Navier–Stokes equations, since they

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more easier satisfy discrete Babuška–Brezzi condition in those applications and secondly, they are easier to handle in our element by element construction of the coarse–grid finite element spaces. In our construction, one computes the coarse–grid stiffness matrices on an element–by–element basis by simple block–elimination of the additional degrees of freedom corresponding to the finer grid space, and thus ending up with a stiffness matrix that have the same sparsity pattern as the original fine–grid stiffness matrix. The algebraic procedure is general, and applies to any nonconforming elements (both in two– and three space dimensions) with nodal degrees of freedom. In general, one can have locally refined meshes, constructed in an adaptive fashion. For such an analysis in the second order selfadjoint coercive case we refer to e.g. Hoppe and Wohlmuth [3]-[4].

In the present report we focus mainly on the construction of the solution scheme based on the algebraic multilevel procedure as explained above.

We consider the diffusion problem

$$\begin{aligned} L\,u = -\nabla(k(x)\,grad\,u) &= f \qquad \text{in } \Omega, \\ u &= g \qquad \text{on } \partial\Omega, \end{aligned} \tag{1.1}$$

where Ω is a given two-dimensional (2D) polygon or a 3D polytope and f is a given sufficiently smooth function on Ω. The bilinear form corresponding to the variational setting of this problem reads as follows

$$a(u,\phi) = \int_\Omega \sum_{i,j} k_{i,j}(x) \frac{\partial u}{\partial x_i} \frac{\partial \phi}{\partial x_j}\, dx.$$

The bounded measurable coefficients $k_{i,j}(x)$ define a symmetric matrix that is assumed to be uniformly positive definite in $x \in \bar{\Omega}$.

Nonconforming finite elements are very attractive for discretizing the Stokes and elasticity problems since they possess favorable stability properties and the divergence–free nodal bases are easily constructed, at least in the 2-D case. A simple nonconforming quadrilateral Stokes element based on *rotated* multi–linear shape functions has been analyzed by Rannacher and Turek in [7] which we use for a decomposition of the domain Ω into convex quadrilaterals (2D). In 3D case convex hexahedrons are used to decompose the domain and nodal rotated basis functions are constructed using the centers of the faces of the finite elements as degrees of freedom. Having constructed the coarse–grid stiffness matrices, and intergrid transfer operators, to apply a standard MG procedure we also need the so–called smoothing procedure. A class of block–ILU factorizations for positive definite block–tridiagonal, not only M–matrices, has been proposed by Chan and Vassilevski [1] and shown to be efficient for certain model computations for systems of differential equations. PCG method with this factorization method we have used as a smoother in the multigrid process used in our numerical experiments..

The remainder of this report is organized as follows. In Section 2, the type of the discretization using rotated multiinear basis functions on quadrilateral and hexahedrons finite elements is described in detail. The essence of our two–grid algebraic procedure of generating the coarse–grid spaces and related matrix–dependent intergrid transfer operators is a topic of consideration in Section 3. Then multilevel method as preconditioner in combination with the PCG method is applied in our global solver. Some computational results on test problems are presented in the last Section 4.

2. Discretization and Assembling

In this section we explain the computation of the element matrix for any finite element T using a discretization of our model domain. Let $\Omega = [0,1] \times [0,1]$ be the unit square and τ be a regular uniform decomposition of Ω into convex quadrilaterals denoted by T. Let the mesh parameter $h > 0$ describe the diameter of the elements of τ. By ∂T we denote the set of all edges Γ of the elements $T \in \tau$.

Consider the reference element $T = [0,h] \times [0,h]$ shown on Figure 1.

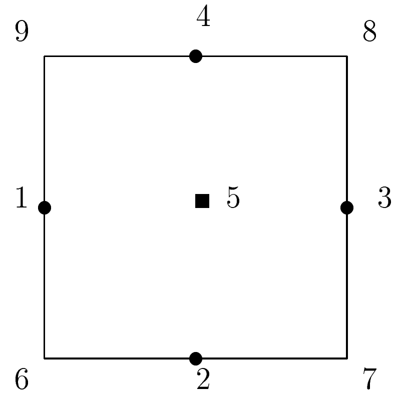

Figure 1. $T = [0,h]\times[0,h]$, h–discretization parameter, $\bullet$ – midpoints of the edges (the grid nodes).

Rotated multi–linear basis functions proposed by Rannacher and Turek [7] are used to construct the nonconforming finite element space. For the corresponding midpoints of the edges these functions have value 1 and they vanish on the remaining midpoints.

For the basis functions

$$\{\phi_i\} \in Span\{1,\ x,\ y,\ x^2 - y^2\}$$

at the nodes i on Figure 1 ($i = 1,2,3,4$) we have the following presentations:

$$\begin{aligned}
\phi_1(x,y) &= -2x/h + y/h + (x^2 - y^2)/h^2 + 3/4 \\
\phi_2(x,y) &= x/h - 2y/h - (x^2 - y^2)/h^2 + 3/4 \\
\phi_3(x,y) &= y/h + (x^2 - y^2)/h^2 - 1/4 \\
\phi_4(x,y) &= x/h - (x^2 - y^2)/h^2 - 1/4.
\end{aligned}$$

As in the standard finite element method, the approximate solution is a linear combination of the basis functions, i.e. $u_h(x,y) = \sum_{i=1}^{n} u_i \phi_i(x,y)$, where the unknown coefficients $\{u_i\}_{i=1}^{n}$ are the desired approximations of the exact solution $u(x,y)$ at the grid nodes and n is the number of all degrees of freedom.

In the local notations, the restriction of the bilinear form over the given finite element T reads as follows:

$$a_T(u_h, \phi_i) = \int_T k\, \nabla u_h \nabla \phi_i \, dT. \tag{2.1}$$

The following quadrature rule exact for polynomials of degree 3 is used to approximate the integrals over the volume T (see Figure 1).

$$\int_T f(x)\,dx = \frac{h^2}{6}\left[\sum_{i=1}^{4} f(i) + 2f(5)\right].$$

Since $\nabla\phi = \left(\frac{\partial\phi}{\partial x}, \frac{\partial\phi}{\partial y}\right)$ for the first derivatives of the basis functions we get

$$\begin{array}{ll}
\partial\phi_1/\partial x = -2/h + 2x/h^2, & \partial\phi_1/\partial y = 1/h - 2y/h^2 \\
\partial\phi_2/\partial x = 1/h - 2x/h^2, & \partial\phi_2/\partial y = -2/h + 2y/h^2 \\
\partial\phi_3/\partial x = 2x/h^2, & \partial\phi_3/\partial y = 1/h - 2y/h^2 \\
\partial\phi_4/\partial x = 1/h - 2x/h^2, & \partial\phi_4/\partial y = 2y/h^2.
\end{array}$$

The corresponding element matrix is symmetric, denoted by $E = \{e_{ij}\}$ for $i, j = 1, \ldots 4$ where $e_{ij} = \int_T k\,\nabla\phi_i \nabla\phi_j\,dT$.

In the three–dimensional space we consider also rotated multilinear basis functions. Let $T = [-h/2, h/2] \times [-h/2, h/2] \times [-h/2, h/2]$ be the reference element and the nodes are chosen to be the centers of its faces, denoted respectively by the points $1(-h/2, 0, 0)$, $2(h/2, 0, 0)$, $3(0, -h/2, 0)$, $4(0, h/2, 0)$, $5(0, 0, -h/2)$ and $6(0, 0, h/2)$. Then the corresponding basis functions have the following presentations:

$$\begin{array}{rcl}
\phi_1(x,y,z) & = & 1/6 - x/h + 4x^2/3h^2 - 2y^2/3h^2 - 2z^2/3h^2 \\
\phi_2(x,y,z) & = & 1/6 + x/h + 4x^2/3h^2 - 2y^2/3h^2 - 2z^2/3h^2 \\
\phi_3(x,y,z) & = & 1/6 - y/h - 2x^2/3h^2 + 4y^2/3h^2 - 2z^2/3h^2 \\
\phi_4(x,y,z) & = & 1/6 + y/h - 2x^2/3h^2 + 4y^2/3h^2 - 2z^2/3h^2 \\
\phi_5(x,y,z) & = & 1/6 - z/h - 2x^2/3h^2 - 2y^2/3h^2 + 4z^2/3h^2 \\
\phi_6(x,y,z) & = & 1/6 + z/h - 2x^2/3h^2 - 2y^2/3h^2 + 4z^2/3h^2
\end{array}$$

For the first derivatives of the basis functions we get

$$\begin{array}{lll}
\partial\phi_1/\partial x = -1/h + 8x/3h^2, & \partial\phi_1/\partial y = -4y/3h^2, & \partial\phi_1/\partial z = -4z/3h^2 \\
\partial\phi_2/\partial x = 1/h + 8x/3h^2, & \partial\phi_2/\partial y = -4y/3h^2, & \partial\phi_2/\partial z = -4z/3h^2 \\
\partial\phi_3/\partial x = -4x/3h^2, & \partial\phi_3/\partial y = -1/h + 8y/3h^2, & \partial\phi_3/\partial z = -4z/3h^2 \\
\partial\phi_4/\partial x = -4x/3h^2, & \partial\phi_4/\partial y = 1/h + 8y/3h^2y, & \partial\phi_4/\partial z = -4z/3h^2 \\
\partial\phi_5/\partial x = -4x/3h^2, & \partial\phi_5/\partial y = -4y/3h^2, & \partial\phi_5/\partial z = -1/h + 4z/3h^2 \\
\partial\phi_6/\partial x = -4x/3h^2, & \partial\phi_6/\partial y = -4y/3h^2, & \partial\phi_6/\partial z = 1/h + 4z/3h^2.
\end{array}$$

3. An Algebraic Two–level Method

In this section we explain the two–level discretization of the domain where the diffusion equation is solved using nonconforming finite elements. Note that for such elements the so obtained fine and coarse finite element spaces are not nested which is the main difficulty realizing the two–level method.

Consider a reference coarse finite element T with a discretization parameter H which consists of four neighbor finite elements from the fine grid denoted on Figure 2 by T_1, T_2, T_3, T_4. The fine discretization parameter is taken $h = H/2$.

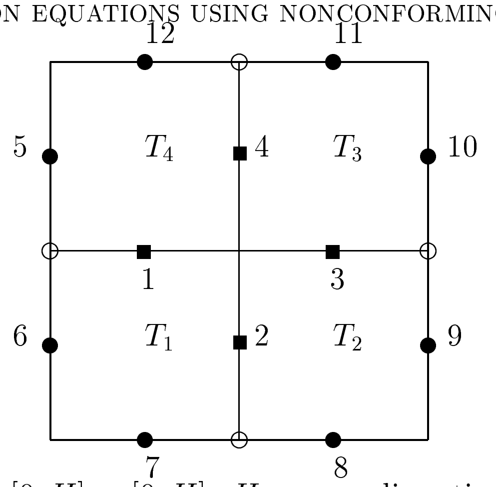

FIGURE 2. $T = [0, H] \times [0, H]$, H–coarse discretization parameter, $T = T_1 \cup T_2 \cup T_3 \cup T_4$, ■ – the interior nodes, ○ – the nodes of the coarse grid finite element T.

Consider the following 12×12 local element matrix

$$A = \begin{bmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{bmatrix}$$

where the first block A_{11} is 4×4 matrix corresponding to the interior nodes $1, 2, 3, 4$ on Figure 2 and the second block A_{22} is of order 8×8 coming from the connections between the exterior nodes on the coarse grid element edges. The off–diagonal blocks A_{12} and A_{21} are rectangular matrices of order 4×8 and 8×4, respectively.

Each iteration step of the standard two–grid method analyzed by Hackbusch [2] consists of pre–smoothing procedure, coarse–grid correction part and possibly post–smoothing part.

Let solve the linear equation $L_h u_h = f_h$ with a right hand side f. One step of the two–grid (h,H) method (computing u_h^{j+1} from u_h^j) proceeds as follows:

(1) Smoothing part I:

- Compute u_h^j by applying ν_1 (≥ 0) steps of a given relaxation method to u_h^j :

$$u_h^j := \text{RELAX}^{\nu_1}(u_h^j, L_h, f_h).$$

(2) Coarse-grid correction part:

- Compute the defect: $d_h^j = f_h - L_h u_h^j$.
- Restrict the defect: $d_H^j := I_h^H d_h^j$.
- Solve exactly on the coarse grid: $L_H v_h^j = d_H^j$.
- Interpolate the correction: $v_h^j := I_H^h v_H^j$.
- Compute the corrected approximation: $u_h^j + v_h^j$.

(3) Smoothing part II:

- Compute u_h^{j+1} by applying ν_2 (≥ 0) steps of a given relaxation method to $u_h^j + v_h^j$:

$$u_h^{j+1} := \text{RELAX}^{\nu_2}(u_h^j + v_h^j, L_h, f_h).$$

For simplicity of the presentation until the end of this section we omit the index j for the number of the two–grid iteration.

Let d_I be a vector of four components corresponding to the interior nodes. Denote also the vectors $d_1 = (d(5), d(7), d(9), d(11))$ and $d_2 = (d(6), d(8), d(10), d(12))$. For the fine–to–coarse transfer the fine residual vector

$$d_h = \begin{bmatrix} d_I \\ d_1 \\ d_2 \end{bmatrix} \text{ has to be restricted to a coarse grid vector } d_H.$$

For this step, a local element harmonic extension of the type

$$\begin{bmatrix} d_1 \\ d_2 \end{bmatrix} = \begin{bmatrix} d_1 \\ d_2 \end{bmatrix} - A_{21} A_{11}^{-1} d_I \tag{3.1}$$

is used. Then the components of the coarse grid vector taken only over the reference finite element T are computed as follows:

$$d_H(i) := d_H(i) + d_1(i) + d_2(i), \qquad \text{for } i = 1, 2, 3, 4.$$

In this way, by construction, we reduce the number of degrees of freedom using local harmonic extensions of the functions inside the finite element. Note that from (3.1) we have to inverse only the matrix A_{11} which is a dense matrix but of small dimension (4×4). In our computations this inverse is computed exactly.

For the interpolation procedure (coarse–to–fine transfer) we find from v_H the vector

$$v_h = \begin{bmatrix} v_I \\ v_1 \\ v_2 \end{bmatrix}, \text{ so that } v_I = -A_{11}^{-1} A_{12} \begin{bmatrix} v_H \\ v_H \end{bmatrix}.$$

For this step the so obtained values of the coarse grid vector v_H at the nodes denoted by "$\circ$" on Figure 2 are considered as values at both sides around the coarse grid node. From a vector with four components we get a vector consisting of 8 components corresponding to the nodes i, $i = 5, \dots, 12$. Then the multiplication by the rectangular matrix A_{12} is well defined and after the action of A_{11}^{-1} we get the values at the interior nodes $1, 2, 3, 4$ which form v_I, the first block component of v_h.

The global vectors coming from the restriction and interpolation procedures are based on the local information for each finite element. The main advantage of this procedure is to construct nested finite element spaces.

Based on the two–grid method we apply multigrid method given in detail in [2]. Each $(l+1)$-grid iteration (for a given level l) consists also of smoothing parts and coarse-grid correction procedure.

4. Numerical Experiments

In this section we present some computational results for solving the equation

$$-\nabla(k(x,y)\, grad\, u) = f, \qquad (x,y) \in \Omega \tag{4.1}$$

using nonconforming finite element method. Suppose that our model domain is the unit square $\Omega = [0,1] \times [0,1]$. The computations have been carried through over a quadrilateral mesh with a discretization parameter $h = 1/n$.

We consider a model problem with an exact solution $u(x,y) = x(1-x)y(1-y)$ and Dirichlet boundary conditions on $\partial\Omega$.

In Table 1 the discrete L_2- norm of the error between the exact and approximate solution and the number of iterations for different constant values of $k(x,y)$ and n are given.

The preconditioned conjugate gradient (PCG) is applied with a stopping criterion

$$(r,r) \leq 10^{-10}(f,f), \tag{4.2}$$

where r is the current residual vector and f is the right-hand side of the equation.

TABLE 1. L_2- norm of the error and number of iterations.

$k\backslash n$	$n=8$	$n=16$	$n=32$	$n=64$
1	3.657-4 (3)	9.195-5 (5)	2.300-5 (10)	5.770-6 (18)
10^{-1}	3.657-4 (3)	9.214-5 (5)	2.297-5 (10)	5.641-6 (18)
10^{-2}	3.657-4 (3)	9.201-5 (6)	2.287-5 (10)	5.945-6 (19)
10^{-3}	3.657-4 (3)	9.199-5 (6)	2.326-5 (11)	5.467-6 (20)
10^{-4}	3.657-4 (3)	9.198-5 (6)	2.291-5 (11)	5.994-6 (23)

Let consider multilevel discretization of Ω with NL the number of levels, ($NL=1$ corresponds to the two–level discretization). We start with the finest level with a mesh parameter $h=1/n,\ n=2^l$ and at each next coarser level the meshsize is doubled. The coarsest grid consists of no less than four finite elements.

For the global iterative solver we apply PCG method with a stopping criterion (4.2). The multigrid iteration described in Section 3 is used as a preconditioner. Since the preconditioner changes at each global iteration we get, in general, a nonlinear mapping. For the pre- and post- smoothers we use again PCG method with $\nu_1=\nu_2=2$ smoothing iterations and for the exact solver on the coarsest level we have the following stopping criterion

$$(r,r) \leq 10^{-8}(f,f),$$

where f is the right hand side coming as an input data solving the equation on the coarsest level.

The results for the multilevel discretization are listed in Table 2 for $k(x,y)=1$.

We report the number of global PCG iterations (denoted by MG_{iter}) using multigrid method as a preconditioner and the number of PCG iterations to solve the problem on the coarsest grid (denoted by CG_{iter}). Note that an average value for the number of iterations on the coarsest grid at each multigrid iterations $i,\ 1\leq i\leq MG_{iter}$ is CG_{iter}/MG_{iter}.

TABLE 2. Number of iterations MG_{iter} and CG_{iter}, $k(x,y)=1,\ n=64$

iter	$NL=1$	$NL=2$	$NL=3$	$NL=4$
MG_{iter}	6	7	11	9
CG_{iter}	55	35	22	9

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