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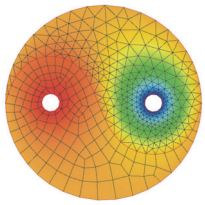

DEALING WITH PERIODIC BOUNDARY CONDITIONS FOR 1D, 2D AND 3D ISOGEOMETRIC FINITE ELEMENT METHOD

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Abstract

In this paper we analyze the problem of implementing periodic boundary conditions in the isogeometric finite element method (ISO-FEM). The ISO-FEM method uses the B-spline-based basis functions, which facilitates usage of the same basis functions for approximation of the geometry as well as for the numerical solution of the modeled physical phenomena. The usage of the B-spline based basis functions results in C^(p-1) global continuity of the solution. The drawback is a difficulty in implementing the periodic boundary conditions, and special dedicated methods are necessary. In this paper we present two algorithms implementing the periodic boundary conditions. The first one is an iterative algorithm that utilizes widely available block-diagonal LAPACK solver. The second one is a modification of the multi-frontal solver algorithm itself, and it requires a dedicated solver with its source code modified accordingly. The presented methods can be applied in one, two or three-dimensional isogeometric finite element method.

Key words: isogeomtric analysis, finite element method, periodic boundary conditions, direct solvers

1. INTRODUCTION

In this paper we discuss some algorithms dealing with periodic boundary conditions for one, two or three-dimensional isogeometric finite element method (IGA-FEM) (Cottrel et al., 2009). The IGA-FEM is a modern method of solving partial differential equations, where the global C^k continuity is kept even on finite element interfaces. This is not the case in classical higher order finite element methods (p-FEM or hp-FEM) where we have only C^0 continuity on finite elements interfaces. The higher continuity of the IGA-FEM is possible to obtain thanks to the utilization of the B-spline basis functions.

However, the B-spline basis functions of order p delivering C^(p-1) continuity have support that spreads over p+1 finite elements. This requires some special treatment in the case of periodic boundary conditions. In this paper we present two algorithms dealing with the periodic boundary conditions for IGA-FEM.

The first algorithm is based on an iterative procedure. It can be summarized in the following way. Periodic boundary conditions induce non-zero terms in heat capacity matrix in the corners outside the main diagonal region. The basic idea is to split this matrix into diagonal and non-diagonal parts, start with solution of the system without non-diagonal part as an initial approximation, and use fixed-point iteration method to obtain successive approximations of the solution. Convergence is linear, each iteration can be reduced to a simple vector equation. Using more sophisticated scheme, faster convergence can be obtained.

The advantage of the first algorithm is that it can be applied using classical, widely available solvers, e.g. LAPACK 2014 solver for block-diagonal matrices for simple 1D geometries (LAPACK, 2014), or

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using Petiga framework, a part of PETSc toolkit. The disadvantage of this algorithm is its iterative nature.

The second algorithm is based on the following simple observation: basically, the boundary conditions can be treated in 1D case as a solution over the 1D circular mesh. In analogous way, we can think of the periodic boundary condition in 2D as a solution over the 2D ball, and in 3D case as a solution over the hyperball. The advantage of this approach is that it can be solved directly, without any iterative procedure. The disadvantage of this approach is that we need to design and implement special solvers for these cases, since classical available solvers, like LAPACK, do not provide such functionality.

2. THE MODEL PROBLEM

Consider the following equation, describing non-stationary heat transport in body with constant density ρ and heat capacity *c*:

$$\rho c \frac{\partial}{\partial t} u = \nabla(\kappa \cdot \nabla u) + f \tag{1}$$

defined on the unit cube $\Omega = (0,1)^3$, with some initial state $u(x,y,z,0) = u_0(x,y,z)$ and periodic boundary conditions, i.e.

$$u(0,y,z,t) = u(1,y,z,t) \tag{2}$$

and similarly for other directions.

Natural way to approach this problem seems to seek solution in a subspace consisting of periodic functions, that is, to choose a periodic basis, for example the tensor product of one-dimensional periodic B-splines, as it is presented in figure 1.

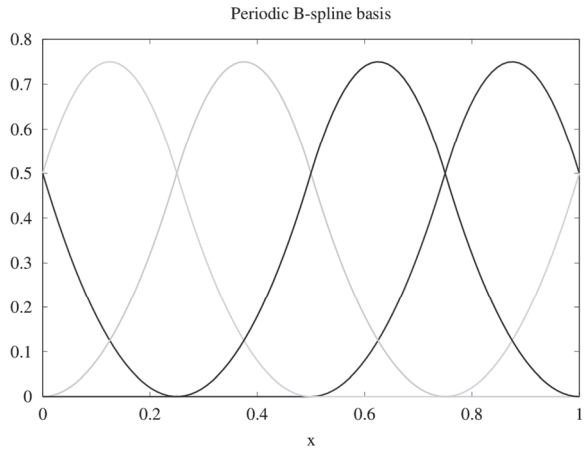

***Fig. 1**. The periodic B-spline basis functions.*

The problem one immediately encounters is the structure of the heat capacity matrix. While in the case of general B-spline basis supports of basic functions are connected and localized in one place, periodic B-splines (or any periodic basis with support not being the whole interval, for that matter) situated "on the edge" have support consisting of two components, at the opposite sides of the interval. This yields additional nonzero entries in the heat capacity matrix, localized in the top right and bottom left corners, while in the usual case the heat capacity matrix is a band matrix. While sufficiently sophisticated specialized solvers can handle the resulting linear equation directly (e.g. the second method described in the paper), lack of banded structure seems to preclude straightforward use of LAPACK.

3. ITERATIVE METHOD

Crucial observation is that usually it should be possible to choose the periodic basis to be similar to an ordinary (non-periodic) one, so that there are not many additional terms in the corner, and the solution to the simplified system, with corner terms omitted, is relatively close to the exact one. This suggests an iterative scheme might be utilized.

For simplicity, let us consider the case of C^0-continuous B-splines (degree 1). In this case, the heat capacity matrix has the banded structure, except for two single entries at the corners. We have

$$M = A + e_1 \otimes e_n + e_n \otimes e_1 \tag{3}$$

where A is banded. We wish to solve the system

$$Mx = b \tag{4}$$

We have thus

$$(A + e_1 \otimes e_n + e_n \otimes e_1)x = b \tag{5}$$

$$x = A^{-1}b - A^{-1}(e_1 \otimes e_n + e_n \otimes e_1)x \tag{6}$$

Let us put $x^{(0)} = A^{-1}b$ (the solution to the simplified system) and $D = A^{-1}(e_1 \otimes e_n + e_n \otimes e_1)$, and iterate

$$x^{(t+1)} = x^{(0)} - Dx^{(t)} \tag{7}$$

D has very simple structure – it is easy to see it has two nonzero columns, first and last, with values $u = A^{-1}e_1$ and $v = A^{-1}e_n$, so the iterative step actually consists of merely two vector-by-scalar multiplications:

$$x^{(t+1)} = x^{(0)} - x_1^{(t)}u - x_n^{(t)}v \tag{8}$$

Generalization is straightforward: heat capacity matrix is split into banded part and the extra terms in the corners, (here $e_1 \otimes e_n + e_n \otimes e_1$), solution to the original system is calculated and used as the first

guess. In general, the number of terms in the above final formula will grow linearly with the number of additional nonzero entries in the corners. In the case of B-spline basis of order p, it means $p(p+1)$ terms. The scheme converges linearly, as shown in figure 2.

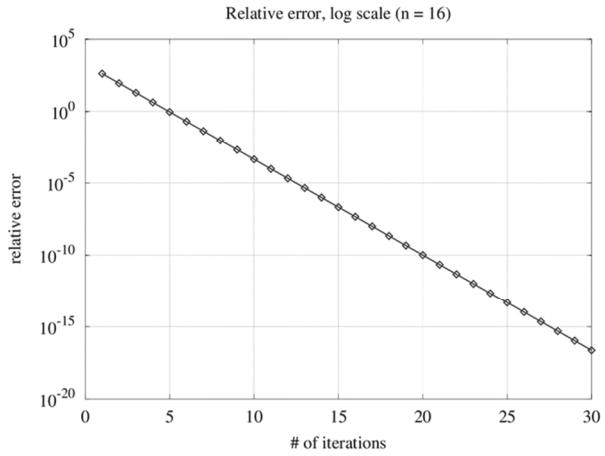

***Fig. 2**. Linear convergence for one of the example projection problems.*

3. CHANGE OF BASIS FUNCTIONS

Sometimes, instead of explicitly using periodic basis, it might be more convenient to compute the heat capacity matrix in simpler basis, and then convert it to the heat capacity matrix corresponding to periodic basis (for example, to utilize existing, efficient code computing the heat capacity matrix for non-periodic basis). This section describes a general way to do this.

Let $\{N_i\}$ be the initial basis, $i = 1, \dots, n$ and $\{\widetilde{N_\iota}\}$ denote the target basis, $i = 1, \dots, m$. Let M be the heat capacity matrix corresponding to the initial basis, that is $M_{ij} = \langle N_i, N_j \rangle$. Assuming the space spanned by $\{\widetilde{N}_i\}$ is a subspace of the one spanned by $\{N_i\}$ (as will usually be the case – in practice, $\{\widetilde{N_\iota}\}$ will span periodic subspace of the full span of $\{N_i\}$), there exists a change-of-basis matrix T, so that

$$\widetilde{N}_j = \sum_{i=1}^{n} T_{ij} N_i \tag{9}$$

Thus, if $\widetilde{\mathrm{M}}$ denotes the heat capacity matrix for $\{\widetilde{N}_i\}$, we have by linearity

$$\widetilde{M}_{ij} = \langle \widetilde{N}_i, \widetilde{N}_j \rangle = \sum_{r,s=1}^{n} T_{ir} T_{js} \langle N_i, N_j \rangle =$$

$$\sum_{s=1}^{n} \left\{ \sum_{r=1}^{n} T_{ir} M_{ij} \right\} T_{js} = [\mathrm{T^T MT}]_{\mathrm{ij}} \tag{10}$$

hence $\widetilde{M} = T^T M T$. Let b be the RHS, that is $b_i = \langle f, N_i \rangle$. Similarly,

$$\tilde{b}_j = \langle f, \widetilde{N}_j \rangle = \sum_{i=1}^{n} T_{ij} \langle f, N_i \rangle = [Tb]_j \tag{11}$$

so $\tilde{b} = Tb$. Therefore, if $T^T M T \tilde{x} = Tb$, then $x = T\tilde{x}$ is the solution to the projection problem posed in the "right" basis - $\{\widetilde{N}_i\}$, expressed in the original basis.

As the bases are most likely fixed and known in advance, T matrix may be precomputed, symbolically or by some numerical method, e.g. by solving system of linear equations arising from evaluating basis functions in suitably chosen set of points. The cost of computation seems negligible compared to the rest of the FEM algorithm, so the method is applicable even if the bases are chosen dynamically.

4. DIRECT METHOD

Let us focus on one dimensional isogeometric finite element method with linear B-splines to discuss the necessary modifications to the solver algorithm when dealing with periodic boundary conditions. In particular, consider knot vector {0,0,1,2,3,4,5,5} and control points {0,1,2,3,4,5} which results in N+2=7 B-spline basis functions. Let us compare the ordinary formulation (zero Dirichlet b.c.) and formulation with periodic b.c. Ordinary formulation yields the following system of equation:

$$\begin{aligned}
&B_1 = 0\\
&B_2 b(N_{3,1}, N_{2,1}) + B_3 b(N_{3,1}, N_{3,1}) + B_4 b(N_{3,1}, N_{4,1}) = f(N_{3,1})\\
&B_3 b(N_{4,1}, N_{3,1}) + B_4 b(N_{4,1}, N_{4,1}) + B_5 b(N_{4,1}, N_{5,1}) = f(N_{4,1})\\
&B_4 b(N_{5,1}, N_{4,1}) + B_5 b(N_{5,1}, N_{5,1}) + B_6 b(N_{5,1}, N_{6,1}) = f(N_{5,1})\\
&B_4 b(N_{6,1}, N_{4,1}) + B_5 b(N_{6,1}, N_{5,1}) + B_6 b(N_{6,1}, N_{6,1}) = f(N_{6,1})\\
&B_7 = 0
\end{aligned} \tag{12}$$

Let us compare the above ordinary formulation with periodic boundary condition formulation:

$$\begin{aligned}
&B_7 b(N_{1,1}, N_{7,1}) + B_1 b(N_{1,1} N_{1,1}) + B_2 b(N_{1,1}, N_{2,1}) = f(N_{1,1})\\
&B_1 b(N_{2,1}, N_{1,1}) + B_2 b(N_{2,1}, N_{2,1}) + B_3 b(N_{2,1}, N_{3,1}) = f(N_{2,1})\\
&B_2 b(N_{3,1}, N_{2,1}) + B_3 b(N_{3,1}, N_{3,1}) + B_4 b(N_{3,1}, N_{4,1}) = f(N_{3,1})\\
&B_3 b(N_{4,1}, N_{3,1}) + B_4 b(N_{4,1}, N_{4,1}) + B_5 b(N_{4,1}, N_{5,1}) = f(N_{4,1})\\
&B_4 b(N_{5,1}, N_{4,1}) + B_5 b(N_{5,1}, N_{5,1}) + B_6 b(N_{5,1}, N_{6,1}) = f(N_{5,1})\\
&B_5 b(N_{6,1}, N_{5,1}) + B_6 b(N_{6,1}, N_{6,1}) + B_1 b(N_{6,1}, N_{1,1}) = f(N_{6,1})
\end{aligned} \tag{13}$$

We can draw the following conclusions from the above example:

- The ordinary (with Dirichlet b.c.) system of linear equations is block-diagonal.
- The block diagonal LAPACK solver can be used in the case of Dirichlet b.c., delivering linear O(N) computational cost.
- The periodic b.c. system is no longer block-diagonal, it has non-zero entries at the top right and bottom left part of the matrix.
- The block diagonal LAPACK solver cannot be used in this case
- The size of the off-diagonal parts in the periodic b.c. case grows when we increase global continuity of the solution, since the support of B-spline basis function of order p spreads over p+1 elements.

Let us recall now the multi-frontal solver approach for solution of the ordinary, non-periodic system so that we can propose the modification to the algorithm for the periodic b.c. case.

Let us assume that we have a simple heat transfer problem u"=1, so the rows of the matrix are equal to [1, -2, 1] after the integration of the weak equations over elements. The multi-frontal solver decomposes the global system into a set of local sub-systems, e.g.

$$\begin{pmatrix}1 & 0\\ 1 & -1\end{pmatrix}\begin{pmatrix}B_1\\ B_2\end{pmatrix}=\begin{pmatrix}0\\ 0.5\end{pmatrix},\begin{pmatrix}-1 & 1\\ 1 & -1\end{pmatrix}\begin{pmatrix}B_2\\ B_3\end{pmatrix}=\begin{pmatrix}0.5\\ 0.5\end{pmatrix},\begin{pmatrix}-1 & 1\\ 1 & -1\end{pmatrix}\begin{pmatrix}B_3\\ B_4\end{pmatrix}=\begin{pmatrix}0.5\\ 0.5\end{pmatrix} \quad (14)$$

$$\begin{pmatrix}-1 & 1\\ 1 & -1\end{pmatrix}\begin{pmatrix}B_4\\ B_5\end{pmatrix}=\begin{pmatrix}0.5\\ 0.5\end{pmatrix},\begin{pmatrix}-1 & 1\\ 1 & -1\end{pmatrix}\begin{pmatrix}B_5\\ B_6\end{pmatrix}=\begin{pmatrix}0.5\\ 0.5\end{pmatrix},\begin{pmatrix}-1 & 1\\ 0 & 1\end{pmatrix}\begin{pmatrix}B_6\\ B_7\end{pmatrix}=\begin{pmatrix}0.5\\ 0\end{pmatrix} \quad (15)$$

We can then merge neighbouring pairs of the systems and eliminate one fully assembled node from each system

$$\begin{pmatrix}-2 & 1 & 1\\ 0 & 1 & 0\\ 1 & 0 & -1\end{pmatrix}\begin{pmatrix}B_2\\ B_1\\ B_3\end{pmatrix}=$$

$$\begin{pmatrix}\vec{0.5}\\ 0\\ 0.5\end{pmatrix},\begin{pmatrix}1 & -1/2 & -1/2\\ 0 & 1 & 0\\ 0 & 1/2 & -1/2\end{pmatrix}\begin{pmatrix}B_2\\ B_1\\ B_3\end{pmatrix}=\begin{pmatrix}-0.25\\ 0\\ 0.75\end{pmatrix} \quad (16)$$

$$\begin{pmatrix}-2 & 1 & 1\\ 1 & -1 & 0\\ 1 & 0 & -1\end{pmatrix}\begin{pmatrix}B_4\\ B_3\\ B_5\end{pmatrix}=$$

$$\begin{pmatrix}\vec{0.5}\\ 0.5\\ 0.5\end{pmatrix},\begin{pmatrix}1 & -1/2 & -1/2\\ 0 & -1/2 & 1/2\\ 0 & 1/2 & -1/2\end{pmatrix}\begin{pmatrix}B_4\\ B_3\\ B_5\end{pmatrix}=\begin{pmatrix}-0.25\\ 0.75\\ 0.75\end{pmatrix} \quad (17)$$

$$\begin{pmatrix}-2 & 1 & 1\\ 1 & -1 & 0\\ 0 & 0 & 1\end{pmatrix}\begin{pmatrix}B_6\\ B_5\\ B_7\end{pmatrix}=$$

$$\begin{pmatrix}\vec{0.5}\\ 0.5\\ 0\end{pmatrix},\begin{pmatrix}1 & -1/2 & -1/2\\ 0 & -1/2 & 1/2\\ 0 & 0 & 0\end{pmatrix}\begin{pmatrix}B_6\\ B_5\\ B_7\end{pmatrix}=\begin{pmatrix}-0.25\\ 0.75\\ 0\end{pmatrix} \quad (18)$$

We end up again with three 2x2 sub-systems, two of them can be merged at this point in the higher level to obtain

$$\begin{pmatrix}-1 & 1/2 & 1/2\\ 0 & 1 & 0\\ 1/2 & 0 & -1/2\end{pmatrix}\begin{pmatrix}B_3\\ B_1\\ B_5\end{pmatrix}=\begin{pmatrix}1.5\\ 0\\ 0.5\end{pmatrix}... \quad (19)$$

Again, we can eliminate the fully assembled first row, and continue this process of partial merging and eliminating up to the root of the tree. The process is followed by recursive backward substitutions.

Let us focus now on the case of the multi-frontal solver algorithm with periodic b.c. The local sub-systems looks like

$$\begin{pmatrix}-1 & 1\\ 1 & -1\end{pmatrix}\begin{pmatrix}B_1\\ B_2\end{pmatrix}=\begin{pmatrix}0.5\\ 0.5\end{pmatrix},\begin{pmatrix}-1 & 1\\ 1 & -1\end{pmatrix}\begin{pmatrix}B_2\\ B_3\end{pmatrix}=\begin{pmatrix}0.5\\ 0.5\end{pmatrix},\begin{pmatrix}-1 & 1\\ 1 & -1\end{pmatrix}\begin{pmatrix}B_3\\ B_4\end{pmatrix}=\begin{pmatrix}0.5\\ 0.5\end{pmatrix} \quad (20)$$

$$\begin{pmatrix}-1 & 1\\ 1 & -1\end{pmatrix}\begin{pmatrix}B_4\\ B_5\end{pmatrix}=\begin{pmatrix}0.5\\ 0.5\end{pmatrix},\begin{pmatrix}-1 & 1\\ 1 & -1\end{pmatrix}\begin{pmatrix}B_5\\ B_6\end{pmatrix}=\begin{pmatrix}0.5\\ 0.5\end{pmatrix},\begin{pmatrix}-1 & 1\\ 1 & -1\end{pmatrix}\begin{pmatrix}B_6\\ B_1\end{pmatrix}=\begin{pmatrix}0.5\\ 0.5\end{pmatrix} \quad (21)$$

Notice that in the last sub-system, there is again B_1 variable. The multi-frontal solver for the case of zero Dirichlet b.c. works over the binary tree structure, but the multi-frontal solver for the case of periodic b.c. works over the binary tree stretched over the 2D circular graph, compare figure 3. The 2D and 3D versions of the multi-frontal solver work in the same way, with the circle replaced by the sphere and hypersphere, respectively.

5. CONCLUSIONS

In this paper we have shown two algorithms, iterative and direct one, for dealing with periodic boundary conditions in the case of isogeometric finite element method computations. The first one has been verified experimentally. The second one requires a straightforward modification of the classical algorithm (Obrok et al., 2010; Wozniak et al., 2014), and it will not alter the computational cost of the multi-frontal solver algorithm (Collier et al., 2012). It is therefore possible to effectively handle such constraints using isogeometric methods. Iterative method, though does not require custom solver,

seems to exhibit rather slow rate of convergence. Using more sophisticated scheme, faster method should be possible to obtain.

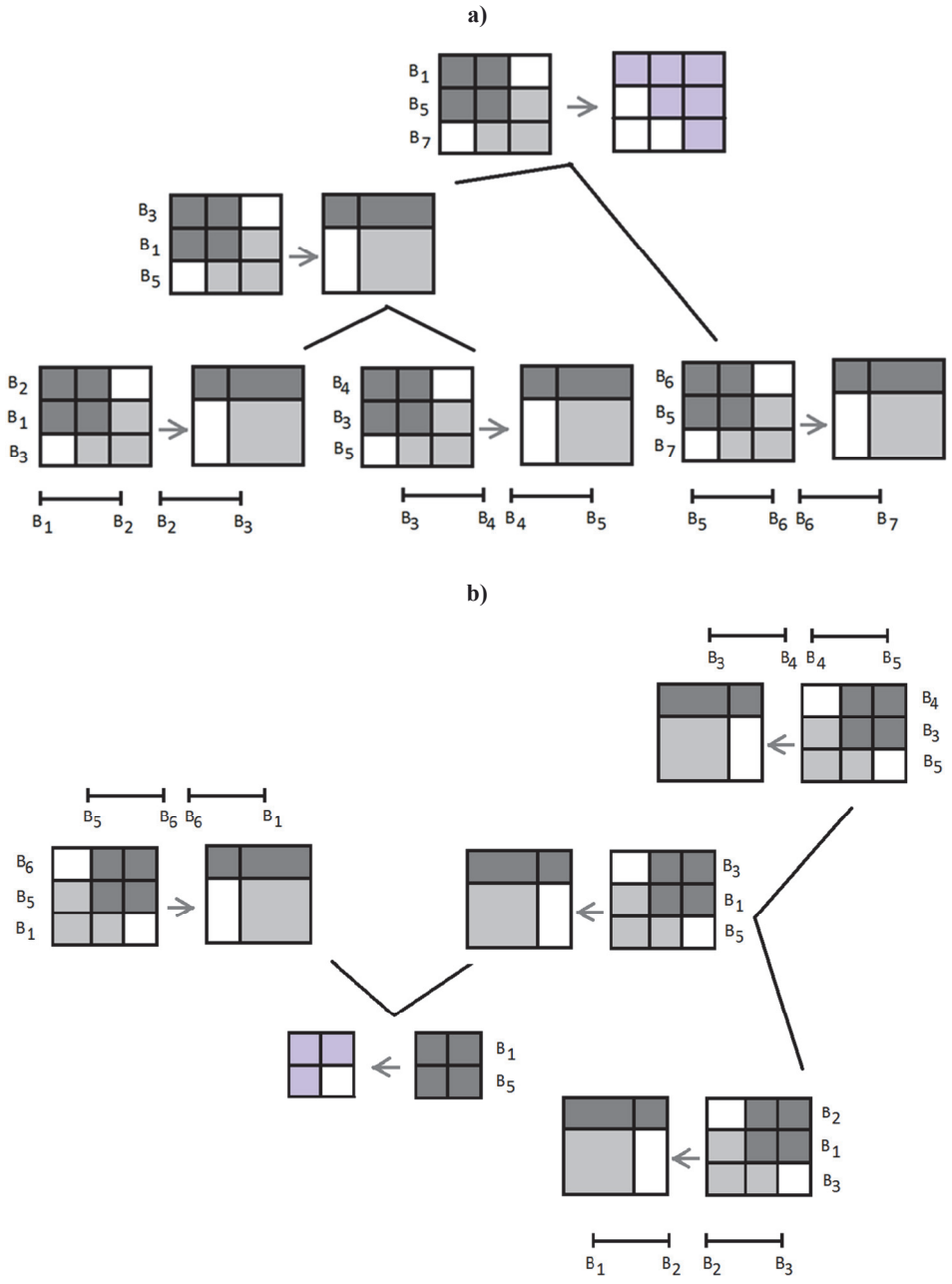

***Fig. 3**. Structure of the multi-frontal solver for Dirichlet b.c. (a) and periodic b.c. (b).*

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IMPLEMENTACJA PERIODYCZNYCH WARUNKÓW BRZEGOWYCH W JEDNO, DWU I TRÓJWYMIAROWEJ IZOGEOMETRYCZNEJ METODZIE ELEMENTÓW SKOŃCZONYCH

Streszczenie

W artykule analizujemy sposób implementacji periodycznych warunków brzegowych w izogeometrycznej metodzie elementów skończonych (ISO-FEM). Metoda ISO-FEM cechuje się użyciem B-spline'ów jako funkcji bazowych, co pozwala na zastosowanie takiej samej bazy wielomianów do odwzorowania geometrii jak również do rozwiązania modelowanego zagadnienia fizycznego. Baza zbudowana z B-spline'ów stopnia p posiada globalną ciągłość C^(p-1). Z tego też powodu sposób wymuszania periodycznych warunków brzegowych nie jest oczywisty, i konieczne jest zastosowanie specjalnych technik. W artykule tym prezentujemy dwa algorytmy wymuszające periodyczne warunki brzegowe. Pierwszy algorytm iteracyjny umożliwia wykorzystanie powszechnie dostępnych solwerów (takich jak LAPACK) dla macierzy blokowo-diagonalnych, drugi algorytm polega na modyfikacji kodu solwera wielofrontalnego, i z tego względu wymaga dedykowanej implementacji algorytmu solwera. Przedstawione sposoby implementacji periodycznych warunków brzegowych można zastosować w jedno, dwu i trójwymiarowej isogeometrycznej metodzie elementów skończonych.

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