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On a construction of fast direct solvers

Applications of Mathematics, Vol. 48 (2003), No. 3, 225–236

Persistent URL: `http://dml.cz/dmlcz/134529`

ON A CONSTRUCTION OF FAST DIRECT SOLVERS

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(Received December 20, 2001)

Abstract. Fast direct solvers for the Poisson equation with homogeneous Dirichlet and Neumann boundary conditions on special triangles and tetrahedra are constructed. The domain given is extended by symmetrization or skew symmetrization onto a rectangle or a rectangular parallelepiped and a fast direct solver is used there. All extendable domains are found. Eigenproblems are also considered.

Keywords: Poisson equation, boundary value problem, fast direct solver, triangle, tetrahedron

MSC 2000: 65F05, 65N22

0. Introduction

In the previous papers [1], [2] we considered the eigenproblem for the Poisson equation with homogeneous Dirichlet or Neumann conditions on the equilateral triangle, both in the continuous and the discrete case. We mentioned there the possibility of the construction of a fast direct solver for the solution of some boundary value problems. The principle was to extend the triangle with angles $\pi/2$, $\pi/3$, $\pi/6$ and a function given on it by symmetrization (for the Neumann boundary condition) and skew symmetrization (for the Dirichlet boundary condition) onto a rectangle. One then uses a fast direct solver on the rectangle and restricts the solution to the original domain.

In the present paper, we consider possible generalizations of this approach to 2 and 3 dimensions and its limitations. In 2 dimensions we find all polygons having the property of covering a rectangle. In 3 dimensions we restrict ourselves to looking for tetrahedra that cover a rectangular parallelepiped. For these domains we show the construction of the fast direct solver and find the eigenfunctions and eigenvalues. We consider only homogeneous boundary conditions and in the sequel all boundary conditions are homogeneous without repeating it each time. The cases of nonhomogeneous boundary conditions are usually solved with a suitably constructed particular solution.

1. Basic definitions

We study problems in 2 and 3 dimensions, these preliminaries being common for both the cases. The term *polytope* will mean a polygon or a polyhedron, the *face* of a polytope will be a side for a polygon or a face for a polyhedron. Moreover, we consider as *faces of lower dimensions* also a vertex in 2 dimensions and an edge or vertex in 3 dimensions. When speaking of a face we understand a face of dimension $d-1$.

The term *movement* in $\mathbb{R}^d$ will mean a transformation T given by the formula $Tx = \mathcal{A}x + b$, where $x \in \mathbb{R}^d$, $\mathcal{A}$ is an orthogonal matrix with $\det \mathcal{A} = 1$ and b a vector. By a *movement with reflection* we denote a transformation of the above form where, however, $\det \mathcal{A} = -1$.

A *covering* of a set D is a system of closed polytopes that cover the set D and whose interiors do not intersect. We restrict ourselves only to coverings with polytopes because each covering of the space with convex sets is a covering with polytopes, Theorem 1, Ch. 3.5 [3].

A covering is a *face to face covering* if the intersection of each pair of polytopes is either empty or a face (possibly of lower dimension) of both the polytopes. We say that two polytopes are *neighbours* if they have a common face.

We say that a face to face covering of the set D is an *R-covering* (generated by a polytope P_1) if

$$D = \bigcup_{i=1}^{K} P_i \quad \text{and} \quad P_i = T_i P_1, \quad i = 1, \ldots, K,$$

where T_i is a movement or a movement with reflection, and for every pair of neighbouring polytopes P_i and P_j, the relation $P_i = TP_j$ holds, where T is a movement with reflection letting the common face pointwise invariant (i.e. we have the common symmetry of P_i and P_j).

The transformations T_i are not uniquely determined. We can, e.g., transform the triangle $(0,0)$, $(1,0)$, $(0,1)$ to the triangle $(1,1)$, $(1,0)$, $(0,1)$ either by T_1 with $A_1 = \begin{pmatrix} -1 & 0 \\ 0 & -1 \end{pmatrix}$ and $b_1^T = (1,1)$ or by T_2 with $A_2 = \begin{pmatrix} 0 & -1 \\ -1 & 0 \end{pmatrix}$ and $b_2^T = b_1^T$. Only T_2 is the above mentioned symmetry.

Our aim is, however, to prolong a function given on P_1 onto D and, therefore, we impose a more severe restriction on the covering.

A covering will be called *prolongable* if it is an R-covering with such transformations T_i that give the above "symmetry" T of neighbouring P_i and P_j exactly as $T = T_i T_j^{-1}$. If we divide all polytopes of a prolongable covering into two classes such that one contains the polytopes which are images of P_1 by movements without reflection and the second the other ones then all neighbours of every polytope of one class belong to the other.

It is easy to show that an R-covering need not be a prolongable covering. In Fig. 1 we have an R-covering of an equilateral triangle with the triangles P_1, P_2, P_3. It is obvious that these triangles cannot be divided into two classes in the above sense. The triangles P_2, P_3 as neighbours belong to different classes but, on the other hand, as neighbours of P_1 they belong to the same class.

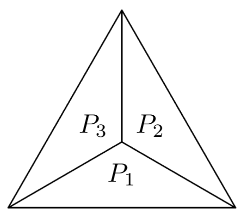

Figure 1. A not prolongable R-covering.

We prolong a function from one polytope to its neighbour by symmetry or skew symmetry. The type of the prolongation depends on the boundary conditions. On each face of P_1 we have either the homogeneous Dirichlet condition corresponding to the skew-symetric prolongation or the homogeneous Neumann condition corresponding to the symmetric prolongation. With each face we therefore associate the number $+1$ or -1, the *boundary type*, for the symmetric and skew-symmetric prolongation, respectively. The set of all boundary types is called *the boundary signature.* The values associated with the faces of P_i will be transferred from the corresponding faces of P_1 by the transformations T_i.

Now, we associate with each polytope P_i a number c_i equal to $+1$ or -1. We put $c_1 = +1$. The set $\{c_1, c_2, \ldots, c_K\}$ is called the *covering signature.* We say that the covering signature is *compatible* with the boundary signature if $c_i = cc_j$ where c is the boundary type of the common face of P_i and P_j.

Moreover, we demand that all faces of the polytopes of a compatible covering lying on one face of D have the same boundary type.

If the boundary signature allows a compatible covering signature then this covering signature is determined uniquely and we call it the induced signature.

We note that for a given prolongable covering and for a given boundary signature, no compatible signature need exist.

The boundary signature shown in Fig. 2, given on one triangle and transferred by the transformations to the inner boundaries of the hexagon, does not allow any compatible signature. The type on the boundary is irrelevant.

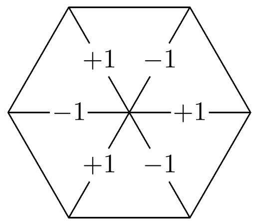

Figure 2. A boundary signature not allowing any compatible covering signature.

Now, let a function $f \in L_2$ be given on P_1. Let a prolongable covering of a rectangular parallepiped and a boundary signature on P_1 be given. Let the induced signature exist. Then we define the prolonged function $F = \mathscr{P} f$ on D by

$$F(B_i) = c_i f(T_i^{-1} B_i), \quad B_i \in P_i, \quad \text{for } i = 1, 2, \ldots, K. \tag{1}$$

The prolongation $\mathscr{P}$ is a transformation of functions defined on P_1 to D. We now define a transformation $\mathscr{Q}$ that is in a certain sense inverse and transforms functions defined on D to functions defined on P_1. Let U be a function defined on D. We set $u_i(T_i^{-1} B_i) = c_i U(B_i)$ for $i = 1, \ldots, K$. The functions u_i are defined on P_1. We finally define $u = \mathscr{Q} U = \sum_{i=1}^{K} u_i$.

Let us consider a boundary value problem

$$-\Delta u + \sigma u = f \quad \text{on } P_1,$$

σ being a nonnegative constant, equipped with Dirichlet or Neumann boundary conditions on each face of one type. If the polytope P_1 generates a prolongable covering and the boundary type admits a compatible covering structure then we prolong the problem onto D. Instead of solving the boundary value problem on P_1 we solve the prolonged boundary value problem on D. We prolong the right-hand side function according to (1). The boundary conditions on the individual faces of D are given by the boundary type of faces of the polytopes lying on this face. All such faces have the same boundary type. For -1 and $+1$ we thus have the Dirichlet and the Neumann boundary condition, respectively. On D we then solve the boundary value problem

$$-\Delta U + \sigma U = F.$$

We define the space $H_b^1(P_1)$ as the space of those functions of $H^1(P_1)$ whose trace vanishes on the faces of P_1 where the Dirichlet boundary condition is prescribed, i.e., where the boundary type is -1. Similarly we define the space $H_b^1(D)$ as the space of those functions of $H^1(D)$ whose trace vanishes on the faces of D where the Dirichlet boundary condition is prescribed. The faces where the Dirichlet condition is prescribed can be in both cases empty. It is easily seen that $\mathscr{Q}V \in H_b^1(P_1)$ for $V \in H_b^1(D)$.

Now, we formulate (for weak solutions) a theorem that is the basis for the method proposed.

Theorem. *Let $f \in L_2(P_1)$ and let $u \in H_b^1(P_1)$ be the solution of the boundary value problem*

$$\int_{P_1} [(\operatorname{grad} u, \operatorname{grad} v) + \sigma(u, v)] \, \mathrm{d}X_1 = \int_{P_1} (f, v) \, \mathrm{d}X_1 \;\; \forall v \in H_b^1(P_1). \tag{2}$$

Then $U = \mathscr{P}u$ is the solution of the boundary value problem on D

$$\int_D [(\operatorname{grad} U, \operatorname{grad} V) + \sigma(U, V)] \, \mathrm{d}X = \int_D (F, V) \, \mathrm{d}X \;\; \forall V \in H_b^1(D). \tag{3}$$

Proof. We start with the left-hand side of (3). We have

$$\begin{aligned}
&\int_D [(\operatorname{grad} U, \operatorname{grad} V) + \sigma(U, V)] \, \mathrm{d}X \\
&= \sum_{i=1}^K \int_{P_i} [(\operatorname{grad} U, \operatorname{grad} V) + \sigma(U, V)] \, \mathrm{d}X_i \\
&= \sum_{i=1}^K \int_{P_1} [(\operatorname{grad} c_i U(X_1), \operatorname{grad} V(X_1)) + \sigma(c_i U(X_1), V(X_1))] \, \mathrm{d}X_1 \\
&= \int_{P_1} [(\operatorname{grad} u, \operatorname{grad} \mathscr{Q}V) + \sigma(u, \mathscr{Q}V)] \, \mathrm{d}X_1,
\end{aligned}$$

where $X_1 = T_i^{-1} X_i$. This is according to (2) equal to $\int_{P_1} (f, \mathscr{Q}V) \, \mathrm{d}X_1$ and from this we finally obtain $\int_D (F, V) \, \mathrm{d}X$.

The prolonged boundary value problem has either a unique solution or a solution which is unique apart from an additive constant. Thus the restriction $U\big|_{P_1}$ solves the original problem or differs from it only by a constant.

Therefore, instead of the numerical solution of the boundary value problem on P_1, we can solve numerically the prolonged problem on D and restrict the numerical solution to P_1. This can be done by a fast direct solver if D is a rectangular parallelepiped, e.g. the solver from [4] based on the use of FFT [5] or the cyclic reduction and factorization [6].

The number of the extra computational operations remains proportional to the number of the unknowns of the original problem on P_1.

2. Two-dimensional case

First, we describe all R-coverings of the plane. It is clear that the full angle 2π must be an integer multiple of the angles of the covering polygon. The angles are therefore of the form $2\pi/n$ with n being an integer greater than 2. We call the number n the *multiplicity* of the angle and we denote the angle by (n). Analogously, the polygon will be denoted by $(n_1, n_2, \ldots, n_k)$, where n_i are the multiplicities of its angles and n_i and n_{i+1} are the neighbouring angles in the proper order. Evidently, $\sum_{i=1}^{k} 1/n_i = \frac{1}{2}(k-2)$.

If the multiplicity is odd we must impose an additional condition that the polygon is symmetric with respect to the axis of the corresponding angle.

An elementary analysis of these conditions gives all R-coverings of the plane, namely:
triangles $(3,12,12)$, $(4,6,12)$, $(4,8,8)$, $(6,6,6)$, quadrangles $(3,4,6,4)$, $(3,6,3,6)$, $(4,4,4,4)$, and a hexagon $(3,3,3,3,3,3)$.

One obtains these 8 cases from the 11 coverings of Laves omitting the pentagons, see [3], Ch. 3.5.

Only four of them, $(4,6,12)$, $(4,8,8)$, $(6,6,6)$ and $(4,4,4,4)$, yield a prolongable covering of the plane (all polygons with angles of odd multiplicity must be omitted). And from them, in addition to the trivial case of the rectangle $(4,4,4,4)$, we have only two that cover the rectangle, triangles $(4,6,12)$ and $(4,8,8)$. Both these polygons generate a prolongable covering. The following figure shows the coverings.

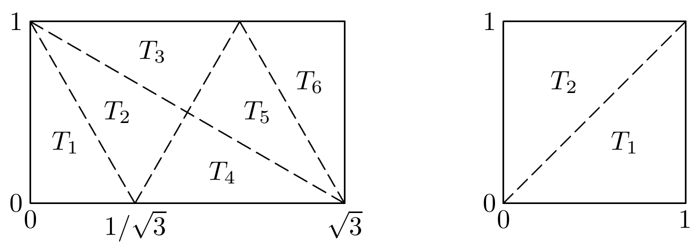

Figure 3. The two coverings of a rectangle.

Triangle $(4, 8, 8)$. Let it have the vertices $(0,0)$, $(1,0)$, $(1,1)$. Then the only non-trivial transformation T_2 onto the triangle $(0,0)$, $(0,1)$, $(1,1)$ has the form $T_2(P) = \mathcal{A}P$, where $\mathcal{A} = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$, the shift is zero.

There is no restriction on boundary conditions in this case. We have 8 possibilities for the choice of the homogeneous Dirichlet or Neumann boundary conditions.

The eigenfunctions of the operator $-\Delta$ on the considered triangle with Dirichlet conditions on all sides are equal to $\sin \pi ix \sin \pi jy - \sin \pi jx \sin \pi iy$ for i, j positive integers with $i < j$. The eigenvalues are $\pi^2(i^2 + j^2)$. The reader easily finds the eigenfunctions for other possible boundary conditions.

Triangle $(4, 6, 12)$. The corresponding transformations for it are shown in [1]. Here we have a restriction on boundary conditions. The boundary conditions on the hypothenuse and the shorter leg of the right angle must be of the same type because they are transformed to the same side of the rectangle.

In the case of the triangle $(4, 6, 12)$ the triangular net is transformed into itself, but the rectangular net is not.

We suppose that the vertices of the triangle are $(0,0)$, $(1/\sqrt{3}, 0)$, $(0,1)$. We give here an illustrative numerical example.

E x a m p l e 1. We solve numerically the same boundary value problem as in [1], $-\Delta u = 2x + 2\sqrt{3}y$ on the triangle $(4, 6, 12)$ with Dirichlet boundary conditions and the exact solution $xy(1 - \sqrt{3}x - y)$. This time on a triangular net, i.e. the points $(ih/\sqrt{3}, jh)$, $i = 1, N-1$, $j = 1, N-i-1$, where $i + j + N \equiv 0 \pmod 2$, $hN = 1$. The problem is extended onto a rectangle and then solved via FFT by the method described in [2]. The results are summarized in Tab. 1.

N	time (s)	time (s)$/N^2 \ln N$	max. error	max. residual
4	8.20E−4	3.70E−5	2.58E−3	4.72E−16
8	3.12E−3	2.34E−5	1.69E−3	2.11E−16
16	1.35E−2	1.90E−5	5.54E−4	1.42E−14
32	5.50E−2	1.55E−5	1.66E−4	6.97E−14
64	2.14E−1	1.26E−5	4.64E−5	6.19E−13
128	9.34E−1	1.17E−5	1.25E−5	2.23E−11
256	3.96	1.09E−5	3.30E−6	7.70E−11
512	28.17	1.72E−5	8.56E−7	4.13E−9
1024	926.92	1.28E−4	2.19E−7	1.24E−8

Table 1. Results of solution of Example 1.

The last two cases are exceptional. They need more time than it is expected. Probably the handling of big arrays is more time consuming on a common PC. The behaviour of the error is as expected. The residuals show a possible influence of round-off errors. The computations have been performed in double precision.

Now, we try to use a fast direct method for this triangle for the construction of fast direct methods for other polygons. The triangle of this type can be prolonged to an equilateral triangle. And it is easily seen that for the choice of Dirichlet or Neumann conditions, the same on all the sides, one can divide the problem into the symmetric and the skew-symmetric problem and solve these problems on the triangle $(4,6,12)$ by a fast direct solver.

3. Three-dimensional case

In this case we study the coverings with tetrahedra only. We start again to look for R-coverings of the whole space.

We have three angles of faces at one vertex. The full angle 2π must be an integer multiple of each angle adjacent to the vertex. Thus, the angles of faces at one vertex are $2\pi/n_1, 2\pi/n_2, 2\pi/n_3$ with positive integers n_1, n_2, n_3, and satisfy in addition the condition $\varepsilon > 0$, where $\varepsilon = 2\pi(1/n_1 + 1/n_2 + 1/n_3) - \pi$ is the spherical excess. We denote the triplet of these angles belonging to one vertex by $[n_1, n_2, n_3]$.

We obtain another condition from the fact that the area of the unit sphere must be an integer multiple of the area of the spherical triangle (equal to the spherical excess).

Under the spherical triangle we understand the intersection of the unit sphere with its center at the vertex with the intersection of three halfspaces each of which is determined by a face meeting the vertex so that it contains the tetrahedron. We have the following condition

$$\frac{1}{n_1} + \frac{1}{n_2} + \frac{1}{n_3} - \frac{1}{2} = \frac{2}{m}$$

where m is a positive integer.

Again, as in the twodimensional case, for an angle of odd multiplicity the spherical triangle must be symmetrical with respect to the plane halving that angle.

Elementary analysis gives the following admissible combinations: $[3,3,3]$, $[3,4,4]$, $[3,6,6]$, $[3,8,8]$, $[3,10,10]$, $[4,6,6]$, $[4,6,8]$, $[4,6,10]$, $[5,5,5]$, $[5,6,6]$ and $[4,4,k]$, $k = 4,5,\ldots$.

We see that only angles with multiplicities 3, 4, 5, 6, 8 and 10 are admissible apart from the case $[4,4,k]$. For all choices of an admissible combination of the angles at a vertex and any two other angles from the above set, we obtained with help of a computer (elementary plane and spherical trigonometry were used) that only the following four tetrahedra are possible as R-coverings of the whole space. The cases $[4,4,k]$ for k different from the above multiplicities are not possible. We thus have:

Tetrahedron T_1. Vertices $A=(0,0,0)$, $B=(1,0,0)$, $C=(1,1,0)$, $D=(1,1,1)$.

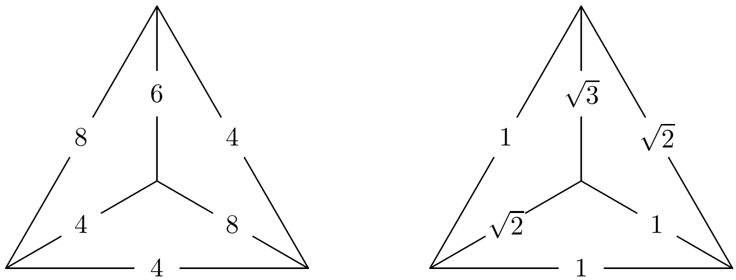

Figure 4. Scheme of angles and edges of the tetrahedron T_1.

Transformations for the covering of the unit cube are $T_i = \mathcal{A}_i P$, where $\mathcal{A}_i$ are the six permutation matrices, $\mathcal{A}_1 = I$, $\mathcal{A}_2 = \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}$, $\mathcal{A}_3 = \begin{pmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix}$, $\mathcal{A}_4 = \begin{pmatrix} 0 & 0 & 1 \\ 0 & 1 & 0 \\ 1 & 0 & 0 \end{pmatrix}$, $\mathcal{A}_5 = \begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{pmatrix}$, $\mathcal{A}_6 = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}$.

There is a restriction here for the choice of the boundary conditions. The conditions on the faces ABD and ACD must be of the same type.

The eigenfunctions of the operator $-\Delta$ with Dirichlet boundary conditions on all faces are

$$\begin{aligned} &\sin i\pi x \sin j\pi y \sin k\pi z - \sin i\pi x \sin k\pi y \sin j\pi z - \sin j\pi x \sin i\pi y \sin k\pi z \\ &+ \sin j\pi x \sin k\pi y \sin i\pi z + \sin k\pi x \sin i\pi y \sin j\pi z - \sin k\pi x \sin j\pi y \sin i\pi z, \end{aligned}$$

i, j, k positive integers with $i<j<k$. The eigenvalues are $\pi^2(i^2+j^2+k^2)$.

We give here an illustrative numerical example.

E x a m p l e 2. We solve numerically the boundary value problem on T_1 for the equation $-\Delta u = f$, where $f = p(x,y,z)\mathrm{e}^{x+y+z}$ and p is a polynomial chosen so that the exact solution is $(1-x)(x-y)(y-z)z\mathrm{e}^{x+y+z}$. The Dirichlet boundary conditions are given on all faces. A uniform cubic net with the step $h=1/N$ was used. This net is transformed by the transformations T_i onto itself. The results are summarized in Tab. 2.

N	time (s)	time (s)$/N^3 \ln N$	max. error	max. residual
8	1.12E−2	1.05E−5	1.45E−4	3.11E−15
16	1.05E−1	9.25E−6	3.89E−5	1.64E−14
32	9.20E−1	8.10E−6	9.80E−6	1.06E−13
48	3.24	7.57E−6	4.36E−6	3.04E−13
64	8.13	7.46E−6	2.45E−6	6.59E−13
80	17.19	7.66E−6	1.57E−6	1.32E−12

Table 2. Results of solution of Example 2.

We have not used extremely big arrays in this example and all results are as is expected and confirm the fast character of the method.

Tetrahedron T_2. Vertices $A = (0,0,0)$, $B = (2,0,0)$, $C = (1,1,0)$, $D = (1,1,1)$.

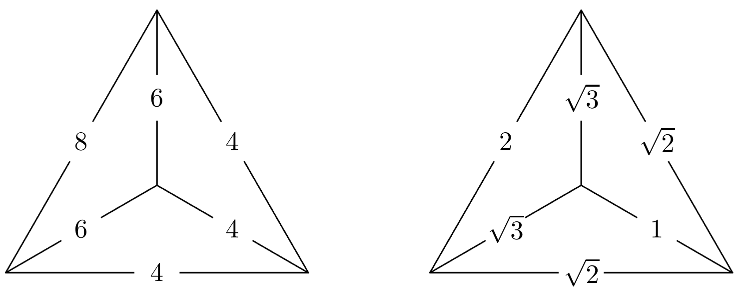

Figure 5. Scheme of angles and edges of the tetrahedron T_2.

This tetrahedron is the union of T_1 and his mirror image. It can be prolonged to the parallelepiped with vertices $(0,0,0)$, $(1,0,1)$, $(1,0,-1)$, $(2,0,0)$, $(0,2,0)$, $(1,2,1)$, $(1,2,-1)$, $(2,2,0)$, twelve pieces necessary, or to the cube with the side equal to 2, 24 pieces necessary.

The fast method for boundary value problems given on it can be constructed with the use of these coverings or by solving the symmetric and skew symmetric parts with a fast method on T_1.

The choice of the boundary conditions is restricted so that the conditions on the faces ABD, ACD, BCD must be of the same type.

The further two tetrahedra are composed from the tetrahedron T_2 in two different ways. They are thus quadruples of the tetrahedron T_1.

Tetrahedron T_3 with the vertices $A = (0,0,0)$, $B = (2,0,0)$, $C = (2,2,0)$, $D = (1,1,1)$.

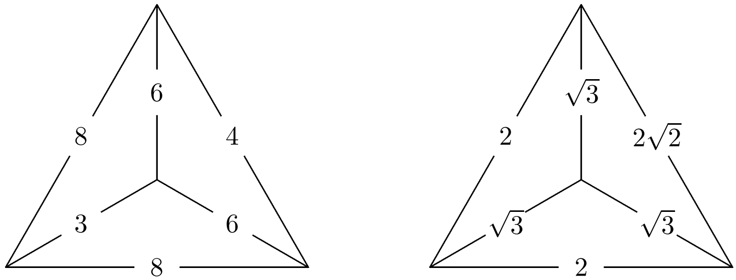

Figure 6. Scheme of angles and edges of the tetrahedron T_3.

This tetrahedron fills the cube (12 pieces are necessary), but the angle of odd multiplicity does not allow a prolongable covering.

Sommerville tetrahedron [7]. Vertices $A = (0,0,0)$, $B = (2,0,0)$, $C = (1,1,1)$, $D = (1,1,-1)$.

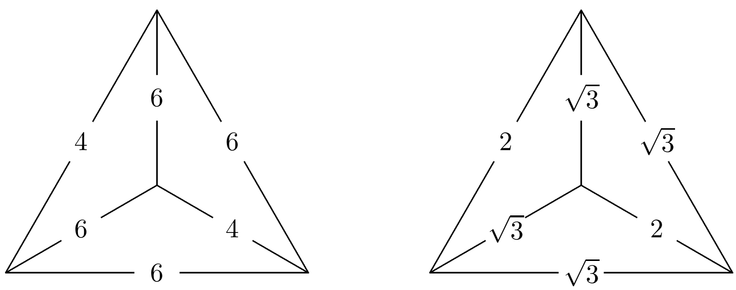

Figure 7. Scheme of angles and edges of the Sommerville tetrahedron.

This tetrahedron fills in the space but not a rectangular parallelepiped.

The boundary value problem given on this tetrahedron under the condition that the boundary conditions on all faces are of the same type can be divided into the symmetric and skew symmetric part and these can be solved on T_2 with a fast method. The eigenfunctions and eigenvalues of the operator $-\Delta$ with such boundary conditions can be given by explicit formulae.

We have shown that the method presented is fast and easy to implement. It can be directly applied to simple problems only but it can be expected that it will be a good preconditioner for more complicated problems defined on domains near to triangle or tetrahedron, especially in the context of the domain decomposition method. It would be interesting to compare it in the future with other methods, the method of fictitious domain or others.

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