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Discretisation of the Maxwell equations on tetrahedral grids

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Abstract

The aim of this report is to describe the discretisation of the Maxwell equations on tetrahedral grids with corresponding dual Voronoi cells to explain the resulting program. The symmetry of the coefficients of the matrix is proven. A small example shows an input file and some other details.

1 The Maxwell equations in the frequency range

For given material constants μ and ε the governing equations in the frequency range are

$$\begin{aligned} \operatorname{rot} \left(\frac{1}{\mu} \mathbf{B} \right) &= j\omega\varepsilon \mathbf{E} \\ \operatorname{rot} (\mathbf{E}) &= -j\omega \mathbf{B} \\ \operatorname{div} (\varepsilon \mathbf{E}) &= 0 \\ \operatorname{div} \mathbf{B} &= 0. \end{aligned}$$

Where \mathbf{E} , \mathbf{B} denote the electrical and magnetic fields, respectively. From these the following integrals can be derived:

$$\begin{aligned} \oint_C \left(\frac{1}{\mu} \mathbf{B} \right) \cdot d\mathbf{s} &= \int_A j\omega\varepsilon \mathbf{E} \cdot d\mathbf{A} \\ \oint_C (\mathbf{E}) \cdot d\mathbf{s} &= \int_A (-j\omega \mathbf{B}) \cdot d\mathbf{A} \\ \oint_S (\varepsilon \mathbf{E}) \cdot \mathbf{n}_S dS &= 0 \\ \oint_S (\mathbf{B}) \cdot \mathbf{n}_S dS &= 0. \end{aligned}$$

Here, A is a finite surface in \mathbb{R}^3 , bounded by a closed curve C , with the vector $d\mathbf{A}$ perpendicular to any point on it, while S denotes the surface of a bounded region with outer normal \mathbf{n}_S , with the vector increment $d\mathbf{s}$ following the course of the curve C in a mathematically positive sense.

2 The electromagnetic field on the grid

For the discretisation, the electrical field strength \mathbf{E} in the centre of the edges and the magnetic induction \mathbf{B} in the circumcentres of the surfaces (triangles) are considered.

Since the field strength and induction only occur within dot products for the integral formulation, they can be restricted to the projection of the electrical field strength to the pertinent edges and the magnetic induction to the pertinent surface-normal.

These projections can be represented as follows:

$$\begin{aligned} P_K(\mathbf{E}(S_{AB})) &= \mathbf{n}_{AB}E_{AB} = \mathbf{n}_{BA}E_{BA} \\ P_N(\mathbf{B}(S_{ABC})) &= \mathbf{n}_{ABC}B_{ABC} = \mathbf{n}_{BCA}B_{BCA} = \mathbf{n}_{CAB}B_{CAB} \\ &= \mathbf{n}_{BAC}B_{BAC} = \mathbf{n}_{ACB}B_{ACB} = \mathbf{n}_{CBA}B_{CBA} \end{aligned}$$

where the following nomenclature has been introduced:

$P_K(\cdot)$	projection on the appropriate edge
$P_N(\cdot)$	projection on the appropriate surface-normal
S_{AB}	centre of the edge AB
S_{ABC}	circumcentre of the triangle ABC
$\mathbf{E}(S_{AB})$	electrical field strength (vector) in S_{AB}
$\mathbf{B}(S_{ABC})$	magnetic induction (vector) in S_{ABC}
\mathbf{n}_{XY}	unit vector in XY direction
\mathbf{n}_{XYZ}	normal vector on the triangle XYZ , which is perpendicular with the mathematically positive sequence of nodes X, Y, Z
E_{XY}, B_{XYZ}	real or complex numbers

(XY or XYZ are permutations of AB or ABC)

The vectors \mathbf{n}_{XY} and \mathbf{n}_{XYZ} clearly satisfy:

$$\begin{aligned} \mathbf{n}_{AB} &= -\mathbf{n}_{BA} \\ \mathbf{n}_{ABC} &= \mathbf{n}_{BCA} = \mathbf{n}_{CAB} = -\mathbf{n}_{BAC} = -\mathbf{n}_{ACB} = -\mathbf{n}_{CBA} \end{aligned}$$

while

$$E_{AB} = -E_{BA} \tag{1}$$

$$B_{ABC} = B_{BCA} = B_{CAB} = -B_{BAC} = -B_{ACB} = -B_{CBA} \tag{2}$$

3 Discretisation of the first Maxwell equation

In the following discretisation of the Maxwell equations, only the favourable case is regarded, all circumcentres of the tetrahedra are situated within the respective tetrahedron.

To discretise the equation

$$\oint_C \left(\frac{1}{\mu} \mathbf{B} \right) \cdot d\mathbf{s} = \int_A j\omega\varepsilon \mathbf{E} \cdot d\mathbf{A},$$

the binary grid (where the nodal points are the circumcentres of the tetrahedra of the primary grid) is employed.

The Voronoi surface of the binary grid (over which one integrates), belongs to the internal edge AB of the primary grid, and is a planar polygon, whose corner points are the circumcentres of all tetrahedra, which possess the common edge AB .

The discretised equation takes the form:

$$\begin{aligned} & \sum_{CD} \frac{1}{\mu_{ABCD}} [l_{ABC}^D \cdot B_{ABC} + l_{ABD}^C \cdot B_{ABD}] \\ &= j\omega \left[\sum_{CD} \frac{1}{2} \varepsilon_{ABCD} (d_{AB}^C \cdot l_{ABC}^D + d_{AB}^D \cdot l_{ABD}^C) \right] E_{AB}, \end{aligned} \quad (3)$$

where the sum is over these tetrahedra $ABCD$, which possess the common edge AB .

$\mu_{ABCD}, \varepsilon_{ABCD}$	material constants in the tetrahedron $ABCD$
l_{ABC}^D	distance of the circumcentre of the tetrahedron $ABCD$ to the triangle ABC
d_{AB}^C	distance of the circumcentre of the triangle ABC to the side AB

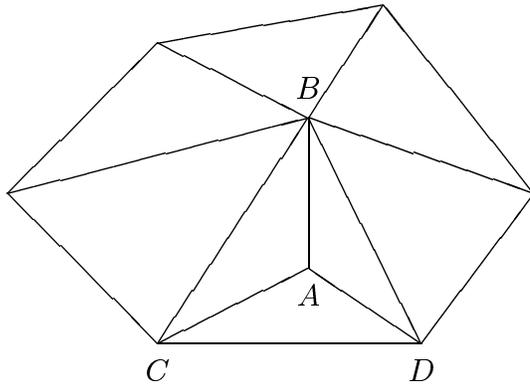


fig.1 Location of the tetrahedra with common edge AB .
The number of tetrahedra must be at least three.

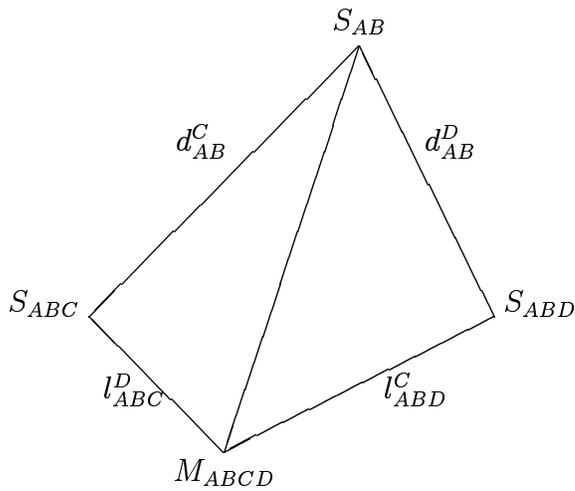


fig.2 Part of the Voronoi surface through the edge AB , to which to the tetrahedron $ABCD$ belongs.

M_{ABCD} circumcentre of the tetrahedron $ABCD$

4 Discretisation of the second Maxwell equation

To discretise

$$\oint_C (\mathbf{E}) \cdot d\mathbf{s} = \int_A (-j\omega \mathbf{B}) \cdot d\mathbf{A},$$

we have employ the primary grid (in contrast to the first Maxwell equation), and integrate over a triangular surface.

This yields the following form:

$$l_{AB} \cdot E_{AB} + l_{BC} \cdot E_{BC} + l_{CA} \cdot E_{CA} = -j\omega B_{ABC} \cdot A_{ABC}, \quad (4)$$

with the associated notation:

l_{AB} length of the distance AB

A_{ABC} area of the triangle ABC

5 Discretisation of the third Maxwell equation

Now we address the first of the surface integrals

$$\oint_S (\varepsilon \mathbf{E}) \cdot \mathbf{n}_S dS = 0,$$

reverting again to the binary grid. It is integrated over the surface of an internal node A of the primary grid to the Voronoi cell. The surface of the Voronoi cell consists of Voronoi surfaces, which belong to edges, whose shared corner node is A . A discretisation formula, similar form to the right-hand side of (3) is obtained,i.e.

$$\sum_B \left(\left[\sum_{CD} \frac{1}{2} \varepsilon_{ABCD} (d_{AB}^C \cdot l_{ABC}^D + d_{AB}^D \cdot l_{ABD}^C) \right] E_{AB} \right) = 0, \quad (5)$$

except now we have an additional outer summation taken over all the nodes of B neighbouring A (in the primary grid).

The summation order in equation (5) can be swapped in the following manner. Within a tetrahedron the node A has exactly three nodes of neighbour. With the calculation the sections which are situated in the tetrahedron $ABCD$ are considered by three different Voronoi surfaces. For the simplification of the representation the equation is multiplied by two.

This leads to the alternative form:

$$\sum_{BCD} (\varepsilon_{ABCD} [(d_{AB}^C \cdot l_{ABC}^D + d_{AB}^D \cdot l_{ABD}^C) E_{AB} + (d_{AC}^B \cdot l_{ABC}^D + d_{AC}^D \cdot l_{ACD}^B) E_{AC} + (d_{AD}^C \cdot l_{ABD}^C + d_{AD}^B \cdot l_{ABD}^C) E_{AD}]) = 0, \quad (6)$$

where now, the summation is over all tetrahedra $ABCD$, which possess the common node A .

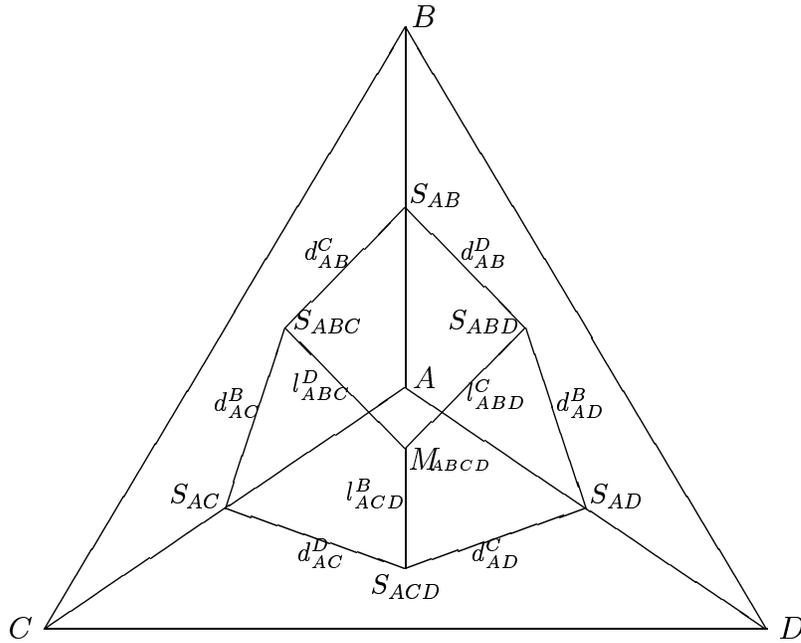


fig.3 Tetrahedron with the proportions of the Voronoi surfaces to the node A

6 Discretisation of the fourth Maxwell equation

For one field integral equation

$$\oint_S (\mathbf{B}) \cdot \mathbf{n}_S dS = 0,$$

the primary grid is again used (as with the second integral equation), only now the integration is over the surface of a tetrahedron.

As a consequence, the discretisation form

$$-A_{ABC} \cdot B_{ABC} - A_{ACD} \cdot B_{ACD} + A_{ABD} \cdot B_{ABD} + A_{BCD} \cdot B_{BCD} = 0 \quad (7)$$

can be deduced.

7 Elimination of the magnetic induction

By multiplying equation (3) by $-j\omega$ and substituting for the variables of type B_{XYZ} in accordance with equation (4), we can deduce that

$$\begin{aligned} & \sum_{CD} \frac{1}{\mu_{ABCD}} \left[\left(\frac{l_{ABC}^D}{A_{ABC}} + \frac{l_{ABD}^C}{A_{ABD}} \right) l_{AB} \cdot E_{AB} + \frac{l_{ABC}^D \cdot l_{BC}}{A_{ABC}} \cdot E_{BC} + \right. \\ & \left. + \frac{l_{ABC}^D \cdot l_{CA}}{A_{ABC}} \cdot E_{CA} + \frac{l_{ABD}^C \cdot l_{BD}}{A_{ABD}} \cdot E_{BD} + \frac{l_{ABD}^C \cdot l_{DA}}{A_{ABD}} \cdot E_{DA} \right] \\ & = \frac{1}{2} \omega^2 \left[\sum_{CD} \varepsilon_{ABCD} (d_{AB}^C \cdot l_{ABC}^D + d_{AB}^D \cdot l_{ABD}^C) \right] E_{AB} \end{aligned} \quad (8)$$

holds, for each internal edge AB of the primary grid. Again here, the summation is taken over those tetrahedra $ABCD$, possessing the common edge AB .

We note that (8) contains only the electric field variables.

8 Graph-theoretical view of the grid

In order to be able to make predictions about the number of variables and the number of equations, the grid is regarded as a graph.

The following notation is used to describe the various geometrical objects which constitute the grid:

E : nodes
 K : edges
 F : surfaces
 T : tetrahedra

E_i : internal nodes
 K_i : internal edges (nodes may exist outside)
 F_i : internal surfaces (nodes and edges may exist outside)

E_0 : nodes of the surface network
 K_0 : edges of the surface network
 F_0 : surfaces of the surface network

A division of the T tetrahedra into T_i internal tetrahedra (all sides are internal surfaces) and T_0 tetrahedra of the surface network (tetrahedron, with which at least one side belongs to the surface network) is not meaningful, since no unique division generally exists.

The following relationships for the grid variables hold:

$$E = E_i + E_0 \tag{9}$$

$$K = K_i + K_0 \tag{10}$$

$$F = F_i + F_0 \tag{11}$$

$$E - K + F - T = 1 \tag{12}$$

$$E_0 - K_0 + F_0 = 2 \tag{13}$$

$$2K_0 = 3F_0 \tag{14}$$

$$4T = 2F_i + F_0 \tag{15}$$

The first set (9) - (11) clearly hold, while the two equations (12) and (13), stem from the Euler polyhedron law for the grid and the surface network. The two remaining equations arise from the following considerations:

Firstly, the surface network is a triangle built from F_0 triangles. These triangles have a total of $3F_0$ edges, but with neighbouring triangles two common edges collapse. Since the network is closed and has no outer edges, equation (14) follows.

Secondly, the T tetrahedra of the grid have $4T$ sides altogether. All inner surfaces belong to exactly two tetrahedra, while each exterior surface belongs to exactly one tetrahedron. Hence, equation (15) holds.

Since we have seven equations with ten variables, then the set of equations is uniquely solvable, providing three of the arguments are known.

Three interesting special cases:

- A) The surface network is determined by providing a single value (E_0, K_0 or F_0), upon solving:

$$(E_0 - K_0 + F_0 = 2) \quad 2K_0 = 3F_0 \quad 2E_0 = 4 + F_0$$

- B) Three values for the grid (three of E, K, F, T) determine the values of the surface network and the internal grid, using:

$$\begin{aligned} E - K + F - T = 1 & \quad F_0 = 2F - 4T & \quad F_i = 4T - F \\ & \quad K_0 = 3F - 6T & \quad K_i = K - 3F + 6T \\ & \quad E_0 = 2 + F - 2T & \quad E_i = E - F + 2T - 2 \end{aligned}$$

- C) With the values for the internal grid (E_i, K_i, F_i) the surface network and the total grid can be deduced from:

$$\begin{aligned} T &= 1 + E_i - K_i + F_i & & \\ K &= 6 + 6E_i - 5K_i + 3F_i & \quad K_0 &= 6 + 6E_i - 6K_i + 3F_i \\ F &= 4 + 4E_i - 4K_i + 3F_i & \quad F_0 &= 4 + 4E_i - 4K_i + 2F_i \\ E &= 4 + 3E_i - 2K_i + F_i & \quad E_0 &= 4 + 2E_i - 2K_i + F_i \end{aligned}$$

9 Reduction of the size of the geometrical constants stemming from the governing equations

The quantities occurring in the discrete form of the Maxwell equations, d_{XY}^Z and l_{XYZ}^W , are unfavourable for computationed purposes. They represent the magnitudes of certain of vector differences and require a square-root operations. This can be avoided however by elimination of the given quantities.

We first define the quantities $V_{ABCM}^D, V_{ABSM}^{CD}$ as follows:

V_{ABCM}^D : Volume of the tetrahedron $ABCM$, whereby M is the circumcentre of the tetrahedron $ABCD$

V_{ABSM}^{CD} : Volume of the tetrahedron $ABSM$, whereby M is the circumcentre of the tetrahedron $ABCD$ and S is the circumcenter of the surface ABC

From these definitions, we can infer that

$$V_{ABCM}^D = \frac{1}{3} \cdot l_{ABC}^D \cdot A_{ABC} \quad (16)$$

$$V_{ABSM}^{CD} = \frac{1}{6} \cdot l_{ABC}^D \cdot d_{AB}^C \cdot l_{AB} \quad (17)$$

hold, and can then use these to substitute for d_{XY}^Z and l_{XYZ}^W in (3),(6) and (8), to get:

$$\begin{aligned} & \sum_{CD} \frac{1}{\mu_{ABCD}} \left[\frac{V_{ABCM}^D}{A_{ABC}} \cdot B_{ABC} + \frac{V_{ABDM}^C}{A_{ABD}} \cdot B_{ABD} \right] \\ &= j\omega \left[\sum_{CD} \varepsilon_{ABCD} \left(\frac{V_{ABSM}^{CD}}{l_{AB}} + \frac{V_{ABSM}^{DC}}{l_{AB}} \right) \right] E_{AB} \end{aligned} \quad (18)$$

$$\begin{aligned} & \sum_{BCD} \left(\varepsilon_{ABCD} \left[\left(\frac{V_{ABSM}^{CD}}{l_{AB}} + \frac{V_{ABSM}^{DC}}{l_{AB}} \right) E_{AB} + \left(\frac{V_{ACSM}^{BD}}{l_{AC}} + \frac{V_{ACSM}^{DB}}{l_{AC}} \right) E_{AC} + \right. \right. \\ & \left. \left. + \left(\frac{V_{ADSM}^{CB}}{l_{AD}} + \frac{V_{ADSM}^{BC}}{l_{AD}} \right) E_{AD} \right] \right) = 0 \end{aligned} \quad (19)$$

$$\begin{aligned} & \sum_{CD} \frac{1}{\mu_{ABCD}} \left[\left(\frac{V_{ABCM}^D}{A_{ABC}^2} + \frac{V_{ABDM}^C}{A_{ABD}^2} \right) l_{AB} \cdot E_{AB} + \frac{V_{ABCM}^D \cdot l_{BC}}{A_{ABC}^2} \cdot E_{BC} + \right. \\ & \left. + \frac{V_{ABCM}^D \cdot l_{CA}}{A_{ABC}^2} \cdot E_{CA} + \frac{V_{ABDM}^C \cdot l_{BD}}{A_{ABD}^2} \cdot E_{BD} + \frac{V_{ABDM}^C \cdot l_{DA}}{A_{ABD}^2} \cdot E_{DA} \right] \\ &= \omega^2 \left[\sum_{CD} \varepsilon_{ABCD} \left(\frac{V_{ABSM}^{CD}}{l_{AB}} + \frac{V_{ABSM}^{DC}}{l_{AB}} \right) \right] E_{AB} \end{aligned} \quad (20)$$

Consequently, to calculate the coefficients in the sets of equations (18), (4), (19), (7) and (20), only the following geometrical sizes of the grid are needed: the circumcentre, the lengths of the edges, the areas of the surfaces, the volume of the tetrahedra, whose nodes are nodes of the network, and the circumcentres of tetrahedra and triangles.

10 Introduction of new variables

Introduction of the variables

$$\mathcal{E}_{AB} = E_{AB} \cdot l_{AB} \quad (21)$$

$$\mathcal{B}_{ABC} = B_{ABC} \cdot A_{ABC} \quad (22)$$

ensures that any „length“ or „surface“ terms of the coefficient of the set of equations (18), (4), (19), (7) and (20) occur only as squares, so that no calculation invoking roots or vector magnitudes is required.

The discrete forms of the four Maxwell equations and the set of equations for the electrical field strengths then be come:

$$\begin{aligned} & \sum_{CD} \frac{1}{\mu_{ABCD}} \left[\frac{V_{ABCM}^D}{A_{ABC}^2} \cdot \mathcal{B}_{ABC} + \frac{V_{ABDM}^C}{A_{ABD}^2} \cdot \mathcal{B}_{ABD} \right] \\ &= j\omega \left[\sum_{CD} \varepsilon_{ABCD} \cdot \frac{V_{ABSM}^{CD} + V_{ABSM}^{DC}}{l_{AB}^2} \right] \mathcal{E}_{AB} \end{aligned} \quad (23)$$

$$\mathcal{E}_{AB} + \mathcal{E}_{BC} + \mathcal{E}_{CA} = -j\omega \cdot \mathcal{B}_{ABC} \quad (24)$$

$$\begin{aligned} & \sum_{BCD} \left(\varepsilon_{ABCD} \left[\frac{V_{ABSM}^{CD} + V_{ABSM}^{DC}}{l_{AB}^2} \cdot \mathcal{E}_{AB} + \frac{V_{ACSM}^{BD} + V_{ACSM}^{DB}}{l_{CA}^2} \cdot \mathcal{E}_{AC} + \right. \right. \\ & \left. \left. + \frac{V_{ADSM}^{CB} + V_{ADSM}^{BC}}{l_{AD}^2} \cdot \mathcal{E}_{AD} \right] \right) = 0 \end{aligned} \quad (25)$$

$$-\mathcal{B}_{ABC} - \mathcal{B}_{ACD} + \mathcal{B}_{ABD} + \mathcal{B}_{BCD} = 0 \quad (26)$$

$$\sum_{CD} \frac{1}{\mu_{ABCD}} \left[\left(\frac{V_{ABCM}^D}{A_{ABC}^2} + \frac{V_{ABDM}^C}{A_{ABD}^2} \right) \mathcal{E}_{AB} + \frac{V_{ABCM}^D}{A_{ABC}^2} \cdot \mathcal{E}_{BC} + \right.$$

$$\begin{aligned}
& + \frac{V_{ABCM}^D}{A_{ABC}^2} \cdot \boldsymbol{\varepsilon}_{CA} + \frac{V_{ABDM}^C}{A_{ABD}^2} \cdot \boldsymbol{\varepsilon}_{BD} + \frac{V_{ABDM}^C}{A_{ABD}^2} \cdot \boldsymbol{\varepsilon}_{DA} \Big] \\
& = \omega^2 \left[\sum_{CD} \varepsilon_{ABCD} \cdot \frac{V_{ABSM}^{CD} + V_{ABSM}^{DC}}{l_{AB}^2} \right] \boldsymbol{\varepsilon}_{AB} \tag{27}
\end{aligned}$$

11 Calculation of the circumcentre of a tetrahedron

The nodes of a non-degenerate tetrahedron are given by the vectors

$$\mathbf{p}_i = (x_i, y_i, z_i)^T, \quad i = 0, 1, 2, 3$$

Also, referring to fig. 4, we define

- F_i : the node \mathbf{p}_i opposite side
- \mathbf{n}_i : normal one at F_i , which is outward arranged concerning the tetrahedron
- h_i : Height of the node \mathbf{p}_i over F_i

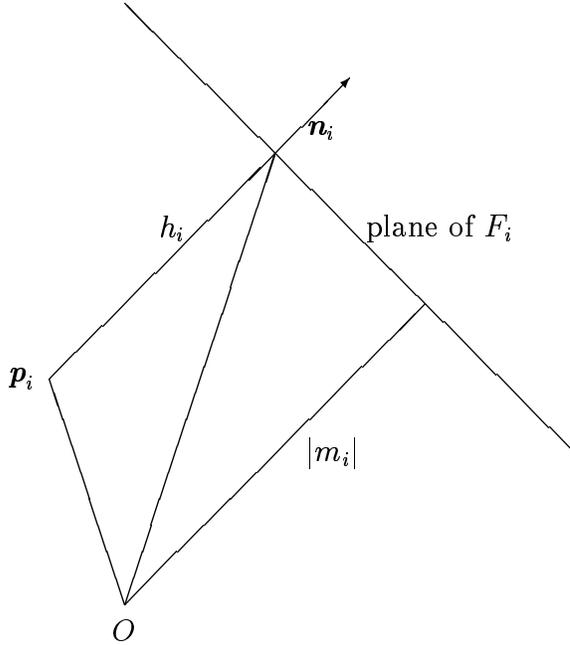


fig. 4 Designations for index i

For all points \mathbf{x} in the plane of F_i , the scalar product with the surface-normal \mathbf{n}_i is constant and has the value m_i , i.e.

$$\mathbf{n}_i \cdot \mathbf{x} = m_i. \quad (28)$$

The value $|m_i|$ is equal to the orthogonal distance of the plane, in which the triangle F_i is situated to the origin.

Furthermore, we note that

$$\mathbf{n}_i \cdot \mathbf{p}_i + h_i = m_i \quad (29)$$

holds, and hence, more generally, we have

$$\mathbf{n}_i \cdot \mathbf{p}_j + h_i \cdot \delta_{ij} = m_i. \quad (30)$$

With $\mathbf{g}_i := -\mathbf{n}_i/h_i$ and $d_i := m_i/h_i$, we rewrite this in the form

$$\mathbf{g}_i \cdot \mathbf{p}_j + d_i = \delta_{ij} \quad i, j = 0, 1, 2, 3 \quad , \quad (31)$$

which is equivalent to the single matrix equation

$$\begin{pmatrix} d_0 & \mathbf{g}_0^T \\ d_1 & \mathbf{g}_1^T \\ d_2 & \mathbf{g}_2^T \\ d_3 & \mathbf{g}_3^T \end{pmatrix} \begin{pmatrix} 1 & 1 & 1 & 1 \\ \mathbf{p}_0 & \mathbf{p}_1 & \mathbf{p}_2 & \mathbf{p}_3 \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \quad (32)$$

To describe further calculations, the following notation is introduced:

\mathbf{M} : circumcentre of the circumsphere

R : radius of the circumsphere

The radius R of the circumsphere satisfies

$$R^2 = (\mathbf{M} - \mathbf{p}_i) \cdot (\mathbf{M} - \mathbf{p}_i) = |\mathbf{M}|^2 - 2\mathbf{p}_i \cdot \mathbf{M} + |\mathbf{p}_i|^2 \quad i = 0, 1, 2, 3. \quad (33)$$

With $\rho := (R^2 - |\mathbf{M}|^2)/2$ it follows that

$$\mathbf{p}_i \cdot \mathbf{M} + \rho = \frac{1}{2}|\mathbf{p}_i|^2 \quad (34)$$

or, in matrix form,

$$\begin{pmatrix} 1 & \mathbf{p}_0^T \\ 1 & \mathbf{p}_1^T \\ 1 & \mathbf{p}_2^T \\ 1 & \mathbf{p}_3^T \end{pmatrix} \begin{pmatrix} \rho \\ \mathbf{M} \end{pmatrix} = \frac{1}{2} \begin{pmatrix} |\mathbf{p}_0|^2 \\ |\mathbf{p}_1|^2 \\ |\mathbf{p}_2|^2 \\ |\mathbf{p}_3|^2 \end{pmatrix} \quad (35)$$

Since the tetrahedra are not degenerate, the matrices are regular in equation (39), and hence invertible, so that

$$\begin{pmatrix} \rho \\ \mathbf{M} \end{pmatrix} = \frac{1}{2} \begin{pmatrix} 1 & \mathbf{p}_0^T \\ 1 & \mathbf{p}_1^T \\ 1 & \mathbf{p}_2^T \\ 1 & \mathbf{p}_3^T \end{pmatrix}^{-1} \begin{pmatrix} |\mathbf{p}_0|^2 \\ |\mathbf{p}_1|^2 \\ |\mathbf{p}_2|^2 \\ |\mathbf{p}_3|^2 \end{pmatrix} = \frac{1}{2} \begin{pmatrix} d_0 & d_1 & d_2 & d_3 \\ \mathbf{g}_0 & \mathbf{g}_1 & \mathbf{g}_2 & \mathbf{g}_3 \end{pmatrix} \begin{pmatrix} |\mathbf{p}_0|^2 \\ |\mathbf{p}_1|^2 \\ |\mathbf{p}_2|^2 \\ |\mathbf{p}_3|^2 \end{pmatrix} \quad (36)$$

holds.

Thus, we have

$$\rho = \frac{1}{2} \sum_{k=0}^3 d_k |\mathbf{p}_k|^2 \quad (37)$$

$$\mathbf{M} = \frac{1}{2} \sum_{k=0}^3 \mathbf{g}_k |\mathbf{p}_k|^2 \quad (38)$$

$$R^2 = |\mathbf{M}|^2 + 2\rho = \frac{1}{4} \sum_{i,k=0}^3 \mathbf{g}_i \cdot \mathbf{g}_k |\mathbf{p}_i|^2 |\mathbf{p}_k|^2 + \sum_{k=0}^3 d_k |\mathbf{p}_k|^2, \quad (39)$$

where, in particular

$$\mathbf{g}_0 = \frac{-\mathbf{n}_0}{h_0} = \frac{-\mathbf{n}_0 \cdot A_{123}}{3V}. \quad (40)$$

12 Calculation of the circumcentre of a triangle

For the calculation of the circumcentre, there are two basic options: It can either be calculated from three vectors of the triangle, or from the projection of the circumcentre of the circumsphere.

In the tetrahedron 0123 \mathbf{g}_0 is located perpendicular to the triangle 123. The constant α , to be determined, is related to the circumcentre \mathbf{S}_{123} by

$$\mathbf{S}_{123} = \mathbf{M} + \alpha \mathbf{g}_0. \quad (41)$$

Since the vector $\mathbf{S}_{123} - \mathbf{p}_i$ is situated in the plane of the triangle 123 for $i = 1, 2, 3$ it must follow that

$$(\mathbf{S}_{123} - \mathbf{p}_i) \cdot \mathbf{g}_0 = 0, \quad (42)$$

for $i = 1, 2, 3$. Choosing $i = 1$, reveals that

$$(\mathbf{M} + \alpha \mathbf{g}_0 - \mathbf{p}_1) \cdot \mathbf{g}_0 = \mathbf{M} \cdot \mathbf{g}_0 + \alpha |\mathbf{g}_0|^2 - \mathbf{p}_1 \cdot \mathbf{g}_0 = 0, \quad (43)$$

so that

$$\alpha = \frac{\mathbf{p}_1 \cdot \mathbf{g}_0 - \mathbf{M} \cdot \mathbf{g}_0}{|\mathbf{g}_0|^2} = \frac{\mathbf{g}_0}{|\mathbf{g}_0|^2} \cdot (\mathbf{p}_1 - \mathbf{M}), \quad (44)$$

and hence,

$$\mathbf{S}_{123} = \mathbf{M} + \frac{\mathbf{p}_1 \cdot \mathbf{g}_0 - \mathbf{M} \cdot \mathbf{g}_0}{|\mathbf{g}_0|^2} \mathbf{g}_0 = \mathbf{M} + \frac{\mathbf{g}_0}{|\mathbf{g}_0|^2} [(\mathbf{p}_1 - \mathbf{M}) \cdot \mathbf{g}_0]. \quad (45)$$

From the equations (45) and (38) it then follows that

$$\mathbf{S}_{123} = \frac{\mathbf{p}_1 \cdot \mathbf{g}_0}{|\mathbf{g}_0|^2} \mathbf{g}_0 + \frac{1}{2} \sum_{k=1}^3 |\mathbf{p}_k|^2 \left(\mathbf{g}_k - \frac{\mathbf{g}_0}{|\mathbf{g}_0|^2} \mathbf{g}_k \cdot \mathbf{g}_0 \right) \quad (46)$$

$$\mathbf{S}_{123} = \frac{1}{2} \sum_{k=0}^3 \left(\mathbf{g}_k |\mathbf{p}_k|^2 - \frac{\mathbf{g}_0}{|\mathbf{g}_0|^2} (\mathbf{g}_0 \cdot \mathbf{g}_k) |\mathbf{p}_k - \mathbf{p}_1|^2 \right). \quad (47)$$

The term in the parentheses of equation (46) is a vector in the plane of the triangle 123, thus \mathbf{S}_{123} is in fact independent of \mathbf{p}_0 .

13 A preconditioner with $graddiv(\varepsilon \mathbf{E})$

From

$$div(\varepsilon \mathbf{E}) = 0 \quad (48)$$

it follows trivially that

$$graddiv(\varepsilon \mathbf{E}) = 0. \quad (49)$$

In order to calculate $graddiv(\varepsilon \mathbf{E})$, we proceed with the definitions of divergence and gradient:

$$div(\varepsilon \mathbf{E}) = \lim_{V \rightarrow 0} \frac{\oint_S (\varepsilon \mathbf{E}) \cdot d\mathbf{S}}{V} \quad (50)$$

$$grad U = \lim_{V \rightarrow 0} \frac{\oint_S U d\mathbf{S}}{V} \quad (51)$$

A discrete form of the divergence is obtained by dividing the appropriate discrete form of the third Maxwell equation with the volume of the pertinent Voronoi cell. The volume V_A for the Voronoi cell surrounding the node A is determined by:

$$V_A = \sum_B \left(\frac{1}{3} \cdot \frac{l_{AB}}{2} \left[\sum_{CD} \frac{1}{2} (d_{AB}^C \cdot l_{ABC}^D + d_{AB}^D \cdot l_{ABD}^C) \right] \right) \quad (52)$$

$$= \frac{1}{2} \sum_B \left[\sum_{CD} (V_{ABSM}^{CD} + V_{ABSM}^{DC}) \right]. \quad (53)$$

Here the first summation is over all neighbouring nodes B of A (in the primary grid) and the second summation is over all tetrahedra, which have the common edge AB .

Also, from equation (6), we have

$$V_A = \frac{1}{12} \sum_{BCD} \left[(d_{AB}^C \cdot l_{ABC}^D + d_{AB}^D \cdot l_{ABD}^C) l_{AB} + (d_{AC}^B \cdot l_{ABC}^D + d_{AC}^D \cdot l_{ACD}^B) l_{AC} + (d_{AD}^C \cdot l_{ACD}^B + d_{AD}^B \cdot l_{ABD}^C) l_{AD} \right] \quad (54)$$

$$V_A = \frac{1}{2} \sum_{BCD} (V_{ABSM}^{CD} + V_{ABSM}^{DC} + V_{ACSM}^{BD} + V_{ACSM}^{DB} + V_{ADSM}^{BC} + V_{ADSM}^{CB}). \quad (55)$$

From equations (19) (divided by two) and (55), we can then deduce a form for the discrete divergence, i.e.

$$\begin{aligned} \text{div}(\varepsilon \mathbf{E}) &= \frac{\sum \varepsilon_{ABCD} \left[(V_{ABSM}^{CD} + V_{ABSM}^{DC}) \frac{E_{AB}}{l_{AB}} + (V_{ACSM}^{BD} + V_{ACSM}^{DB}) \frac{E_{AC}}{l_{AC}} \right]}{\sum (V_{ABSM}^{CD} + V_{ABSM}^{DC} + V_{ACSM}^{BD} + V_{ACSM}^{DB} + V_{ADSM}^{BC} + V_{ADSM}^{CB})} \\ &+ \frac{\sum \varepsilon_{ABCD} \left[(V_{ADSM}^{CB} + V_{ADSM}^{BC}) \frac{E_{AD}}{l_{AD}} \right]}{\sum (V_{ABSM}^{CD} + V_{ABSM}^{DC} + V_{ACSM}^{BD} + V_{ACSM}^{DB} + V_{ADSM}^{BC} + V_{ADSM}^{CB})} \end{aligned} \quad (56)$$

In equations (54) to (56), the summation is over all tetrahedra $ABCD$, possessing the common node A , the divergence of $\varepsilon \mathbf{E}$ in the last equation is over all internal nodes of the primary grid.

For the gradient along the edge AB , we have

$$\text{grad div}(\varepsilon \mathbf{E}) \cdot n_{AB} = \frac{\text{div}(\varepsilon \mathbf{E})_B - \text{div}(\varepsilon \mathbf{E})_A}{|(\mathbf{p}_B - \mathbf{p}_A)|} \quad (57)$$

14 General formula for \mathbf{g}_i

In accordance with equation (47), \mathbf{g}_i is the surface vector located inside the tetrahedron of the surface F_i divided by the volume of the tetrahedron, i.e. the quotient from a suitable cross product and a related triple product.

$$\mathbf{g}_0 = \frac{(\mathbf{p}_1 - \mathbf{p}_3) \times (\mathbf{p}_2 - \mathbf{p}_3)}{(\mathbf{p}_0 - \mathbf{p}_3) \cdot [(\mathbf{p}_1 - \mathbf{p}_3) \times (\mathbf{p}_2 - \mathbf{p}_3)]} \quad (58)$$

This formula applies to all tetrahedra.

The formulae for \mathbf{g}_i with $i = 1, 2, 3$ follow from cyclic permutation of the indices.

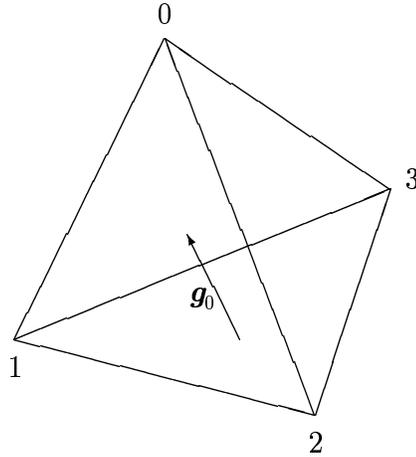


fig.5 Tetrahedron 0123 with vector \mathbf{g}_0

15 Calculation of the coefficient matrix without neighbourhood „knowledge“

From the equation

$$\begin{aligned}
& \sum_{CD} \frac{1}{\mu_{ABCD}} \left[\left(\frac{V_{ABCM}^D}{A_{ABC}^2} + \frac{V_{ABDM}^C}{A_{ABD}^2} \right) \mathcal{E}_{AB} + \frac{V_{ABCM}^D}{A_{ABC}^2} \cdot \mathcal{E}_{BC} + \right. \\
& \left. + \frac{V_{ABCM}^D}{A_{ABC}^2} \cdot \mathcal{E}_{CA} + \frac{V_{ABDM}^C}{A_{ABD}^2} \cdot \mathcal{E}_{BD} + \frac{V_{ABDM}^C}{A_{ABD}^2} \cdot \mathcal{E}_{DA} \right] \\
& = \omega^2 \left[\sum_{CD} \varepsilon_{ABCD} \cdot \frac{V_{ABSM}^{CD} + V_{ABSM}^{DC}}{l_{AB}^2} \right] \mathcal{E}_{AB}, \tag{59}
\end{aligned}$$

we can write

$$M \cdot \mathcal{E} = 0 \tag{60}$$

where:

$$\begin{aligned}
M &= (m_{ij}) && \text{coefficient matrix of the type } (K_i, K - K_{00}) \\
\mathcal{E} &= (\mathcal{E}_i) && \text{variable matrix (column vector) of the type } (K_i, 1)
\end{aligned}$$

Here, the following applies for the variables \mathcal{E}_i ,

$$\mathcal{E}_i = \mathcal{E}_{XY} = l_{XY} \cdot E_{XY}, \tag{61}$$

where the node number of node Y is greater than that of the node X , and the index i is uniquely assigned to the edges XY of the grid:

$$i = k(X, Y). \tag{62}$$

Now it is possible to calculate the entries in the coefficient matrix M without the knowledge of neighbourhood connectivity between the individual tetrahedra.

Furthermore, the tetrahedra of the grid are treated in sequence.

In general, (K_0, K_1, K_2, K_3) is a non-degenerate tetrahedron of the grid with ascending node number K_i ; corresponding vectors are $\mathbf{p}_0, \mathbf{p}_1, \mathbf{p}_2, \mathbf{p}_3$.

The triple product

$$SP = (\mathbf{p}_1 - \mathbf{p}_0) \cdot [(\mathbf{p}_2 - \mathbf{p}_0) \times (\mathbf{p}_3 - \mathbf{p}_0)] \tag{63}$$

is first formed.

As a function of the sign on SP , we apply the following convention:

$$SP > 0 : \quad o = +1 \quad A = K_0 \quad B = K_1 \quad C = K_2 \quad D = K_3 \tag{64}$$

$$SP < 0 : \quad o = -1 \quad A = K_0 \quad B = K_1 \quad C = K_3 \quad D = K_2. \quad (65)$$

Hence, for the vectors, we have

$$SP > 0 : \quad \mathbf{p}_A = \mathbf{p}_0 \quad \mathbf{p}_B = \mathbf{p}_1 \quad \mathbf{p}_C = \mathbf{p}_2 \quad \mathbf{p}_D = \mathbf{p}_3 \quad (66)$$

$$SP < 0 : \quad \mathbf{p}_A = \mathbf{p}_0 \quad \mathbf{p}_B = \mathbf{p}_1 \quad \mathbf{p}_C = \mathbf{p}_3 \quad \mathbf{p}_D = \mathbf{p}_2 \quad (67)$$

In both cases $ABCD$ is a right tetrahedron.

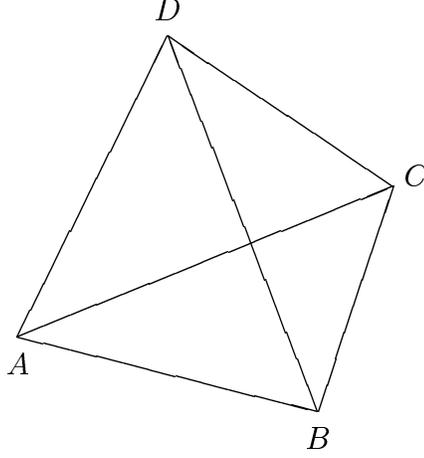


fig.6 Right tetrahedron $ABCD$

Important measures of the tetrahedron can now be categorised.

The edge vectors are

$$\mathbf{p}_{AB} = \mathbf{p}_B - \mathbf{p}_A \quad \mathbf{p}_{AC} = \mathbf{p}_C - \mathbf{p}_A \quad \mathbf{p}_{AD} = \mathbf{p}_D - \mathbf{p}_A \quad (68)$$

$$\mathbf{p}_{BC} = \mathbf{p}_C - \mathbf{p}_B \quad \mathbf{p}_{BD} = \mathbf{p}_D - \mathbf{p}_B \quad \mathbf{p}_{CD} = \mathbf{p}_D - \mathbf{p}_C \quad (69)$$

The surface vectors (directed inwards) are

$$\mathbf{A}_{BCD} = \frac{1}{2} \cdot (\mathbf{p}_{BD} \times \mathbf{p}_{BC}) \quad (70)$$

$$\mathbf{A}_{ACD} = \frac{1}{2} \cdot (\mathbf{p}_{AC} \times \mathbf{p}_{AD}) \quad (71)$$

$$\mathbf{A}_{ABD} = \frac{1}{2} \cdot (\mathbf{p}_{AD} \times \mathbf{p}_{AB}) \quad (72)$$

$$\mathbf{A}_{ABC} = \frac{1}{2} \cdot (\mathbf{p}_{AB} \times \mathbf{p}_{AC}) \quad (73)$$

The volume is

$$V = \frac{1}{3} \cdot (\mathbf{p}_{AB} \cdot \mathbf{A}_{ACD}) \quad (74)$$

The vectors \mathbf{g}_X are

$$\mathbf{g}_A = \frac{\mathbf{A}_{BCD}}{3V} \quad (75)$$

$$\mathbf{g}_B = \frac{\mathbf{A}_{ACD}}{3V} \quad (76)$$

$$\mathbf{g}_C = \frac{\mathbf{A}_{ABD}}{3V} \quad (77)$$

$$\mathbf{g}_D = \frac{\mathbf{A}_{ABC}}{3V} \quad (78)$$

The circumcentre of the circumsphere is

$$\mathbf{M} = \frac{1}{2} \cdot (\mathbf{g}_A |\mathbf{p}_A|^2 + \mathbf{g}_B |\mathbf{p}_B|^2 + \mathbf{g}_C |\mathbf{p}_C|^2 + \mathbf{g}_D |\mathbf{p}_D|^2) \quad (79)$$

The circumcentres of the triangles are

$$\mathbf{S}_{BCD} = \mathbf{M} + \frac{\mathbf{g}_A}{|\mathbf{g}_A|^2} [(\mathbf{p}_B - \mathbf{M}) \cdot \mathbf{g}_A] \quad (80)$$

$$\mathbf{S}_{ACD} = \mathbf{M} + \frac{\mathbf{g}_B}{|\mathbf{g}_B|^2} [(\mathbf{p}_A - \mathbf{M}) \cdot \mathbf{g}_B] \quad (81)$$

$$\mathbf{S}_{ABD} = \mathbf{M} + \frac{\mathbf{g}_C}{|\mathbf{g}_C|^2} [(\mathbf{p}_A - \mathbf{M}) \cdot \mathbf{g}_C] \quad (82)$$

$$\mathbf{S}_{ABC} = \mathbf{M} + \frac{\mathbf{g}_D}{|\mathbf{g}_D|^2} [(\mathbf{p}_A - \mathbf{M}) \cdot \mathbf{g}_D] \quad (83)$$

The volumes of the tetrahedra, based on one side and the circumcentre of the circumsphere, are

$$V_{ABCM}^D = V_{ABCM} = \frac{1}{3} \cdot [\mathbf{A}_{ABC} \cdot (\mathbf{M} - \mathbf{p}_A)] \quad (84)$$

$$V_{ABDM}^C = V_{ABDM} = \frac{1}{3} \cdot [\mathbf{A}_{ABD} \cdot (\mathbf{M} - \mathbf{p}_A)] \quad (85)$$

$$V_{ACDM}^B = V_{ACDM} = \frac{1}{3} \cdot [\mathbf{A}_{ACD} \cdot (\mathbf{M} - \mathbf{p}_A)] \quad (86)$$

$$V_{BCDM}^A = V_{BCDM} = \frac{1}{3} \cdot [\mathbf{A}_{BCD} \cdot (\mathbf{M} - \mathbf{p}_B)] \quad (87)$$

The volumes of the tetrahedra, based on an edge, a circumcentre of a triangle and the circumcentre of the circumsphere, are

$$V_{ABSM}^{CD} = V_{ABS_{ABC}M} = \frac{1}{6} \cdot \mathbf{p}_{AB} \cdot [(\mathbf{S}_{ABC} - \mathbf{p}_A) \times (\mathbf{M} - \mathbf{p}_A)] \quad (88)$$

$$V_{ABSM}^{DC} = V_{ABS_{ABD}M} = -\frac{1}{6} \cdot \mathbf{p}_{AB} \cdot [(\mathbf{S}_{ABD} - \mathbf{p}_A) \times (\mathbf{M} - \mathbf{p}_A)] \quad (89)$$

$$V_{ACSM}^{BD} = V_{ACS_{ABC}M} = -\frac{1}{6} \cdot \mathbf{p}_{AC} \cdot [(\mathbf{S}_{ABC} - \mathbf{p}_A) \times (\mathbf{M} - \mathbf{p}_A)] \quad (90)$$

$$V_{ACSM}^{DB} = V_{ACS_{ACD}M} = \frac{1}{6} \cdot \mathbf{p}_{AC} \cdot [(\mathbf{S}_{ACD} - \mathbf{p}_A) \times (\mathbf{M} - \mathbf{p}_A)] \quad (91)$$

$$V_{ADSM}^{BC} = V_{ADS_{ABD}M} = \frac{1}{6} \cdot \mathbf{p}_{AD} \cdot [(\mathbf{S}_{ABD} - \mathbf{p}_A) \times (\mathbf{M} - \mathbf{p}_A)] \quad (92)$$

$$V_{ADSM}^{CB} = V_{ADS_{ACD}M} = -\frac{1}{6} \cdot \mathbf{p}_{AD} \cdot [(\mathbf{S}_{ACD} - \mathbf{p}_A) \times (\mathbf{M} - \mathbf{p}_A)] \quad (93)$$

$$V_{BCSM}^{AD} = V_{BCS_{ABC}M} = \frac{1}{6} \cdot \mathbf{p}_{BC} \cdot [(\mathbf{S}_{ABC} - \mathbf{p}_B) \times (\mathbf{M} - \mathbf{p}_B)] \quad (94)$$

$$V_{BCSM}^{DA} = V_{BCS_{BCD}M} = -\frac{1}{6} \cdot \mathbf{p}_{BC} \cdot [(\mathbf{S}_{BCD} - \mathbf{p}_B) \times (\mathbf{M} - \mathbf{p}_B)] \quad (95)$$

$$V_{BDSM}^{AC} = V_{BDS_{ABD}M} = -\frac{1}{6} \cdot \mathbf{p}_{BD} \cdot [(\mathbf{S}_{ABD} - \mathbf{p}_B) \times (\mathbf{M} - \mathbf{p}_B)] \quad (96)$$

$$V_{BDSM}^{CA} = V_{BDS_{BCD}M} = \frac{1}{6} \cdot \mathbf{p}_{BD} \cdot [(\mathbf{S}_{BCD} - \mathbf{p}_B) \times (\mathbf{M} - \mathbf{p}_B)] \quad (97)$$

$$V_{CDSM}^{AB} = V_{CDS_{ACD}M} = \frac{1}{6} \cdot \mathbf{p}_{CD} \cdot [(\mathbf{S}_{ACD} - \mathbf{p}_C) \times (\mathbf{M} - \mathbf{p}_C)] \quad (98)$$

$$V_{CDSM}^{BA} = V_{CDS_{BCD}M} = -\frac{1}{6} \cdot \mathbf{p}_{CD} \cdot [(\mathbf{S}_{BCD} - \mathbf{p}_C) \times (\mathbf{M} - \mathbf{p}_C)] \quad (99)$$

Now we have the required information to solve equation (59) for all six (arranged) edges of the tetrahedron provided they are inner edges of the grid:

$$\begin{aligned} & \sum_{CD} \frac{1}{\mu_{ABCD}} \left[\left(\frac{V_{ABCM}^D}{A_{ABC}^2} + \frac{V_{ABDM}^C}{A_{ABD}^2} \right) \boldsymbol{\varepsilon}_{AB} + \frac{V_{ABCM}^D}{A_{ABC}^2} \cdot \boldsymbol{\varepsilon}_{BC} - \right. \\ & \left. - \frac{V_{ABCM}^D}{A_{ABC}^2} \cdot \boldsymbol{\varepsilon}_{AC} + \frac{V_{ABDM}^C}{A_{ABD}^2} \cdot \boldsymbol{\varepsilon}_{BD} - \frac{V_{ABDM}^C}{A_{ABD}^2} \cdot \boldsymbol{\varepsilon}_{AD} \right] \\ & = \omega^2 \left[\sum_{CD} \boldsymbol{\varepsilon}_{ABCD} \cdot \frac{V_{ABSM}^{CD} + V_{ABSM}^{DC}}{l_{AB}^2} \right] \boldsymbol{\varepsilon}_{AB} \end{aligned} \quad (100)$$

$$\begin{aligned}
& \sum_{DB} \frac{1}{\mu_{ABCD}} \left[\left(\frac{V_{ACDM}^B}{A_{ACD}^2} + \frac{V_{ABCM}^D}{A_{ABC}^2} \right) \mathcal{E}_{AC} + \frac{V_{ACDM}^B}{A_{ACD}^2} \cdot \mathcal{E}_{CD} - \right. \\
& \left. - \frac{V_{ACDM}^B}{A_{ACD}^2} \cdot \mathcal{E}_{AD} - \frac{V_{ABCM}^D}{A_{ABC}^2} \cdot \mathcal{E}_{BC} - \frac{V_{ABCM}^D}{A_{ABC}^2} \cdot \mathcal{E}_{AB} \right] \\
& = \omega^2 \left[\sum_{DB} \varepsilon_{ABCD} \cdot \frac{V_{ACSM}^{DB} + V_{ACSM}^{BD}}{l_{AC}^2} \right] \mathcal{E}_{AC} \tag{101}
\end{aligned}$$

$$\begin{aligned}
& \sum_{BC} \frac{1}{\mu_{ABCD}} \left[\left(\frac{V_{ABDM}^C}{A_{ABD}^2} + \frac{V_{ACDM}^B}{A_{ACD}^2} \right) \mathcal{E}_{AD} - \frac{V_{ABDM}^C}{A_{ABD}^2} \cdot \mathcal{E}_{BD} - \right. \\
& \left. - \frac{V_{ABDM}^C}{A_{ABD}^2} \cdot \mathcal{E}_{AB} - \frac{V_{ACDM}^B}{A_{ACD}^2} \cdot \mathcal{E}_{CD} - \frac{V_{ACDM}^B}{A_{ACD}^2} \cdot \mathcal{E}_{AC} \right] \\
& = \omega^2 \left[\sum_{BC} \varepsilon_{ABCD} \cdot \frac{V_{ADSM}^{BC} + V_{ADSM}^{CB}}{l_{AD}^2} \right] \mathcal{E}_{AD} \tag{102}
\end{aligned}$$

$$\begin{aligned}
& \sum_{AD} \frac{1}{\mu_{ABCD}} \left[\left(\frac{V_{ABCM}^D}{A_{ABC}^2} + \frac{V_{BCDM}^A}{A_{BCD}^2} \right) \mathcal{E}_{BC} - \frac{V_{ABCM}^D}{A_{ABC}^2} \cdot \mathcal{E}_{AC} + \right. \\
& \left. + \frac{V_{ABCM}^D}{A_{ABC}^2} \cdot \mathcal{E}_{AB} + \frac{V_{BCDM}^A}{A_{BCD}^2} \cdot \mathcal{E}_{CD} - \frac{V_{BCDM}^A}{A_{BCD}^2} \cdot \mathcal{E}_{BD} \right] \\
& = \omega^2 \left[\sum_{AD} \varepsilon_{ABCD} \cdot \frac{V_{BCSM}^{AD} + V_{BCSM}^{DA}}{l_{BC}^2} \right] \mathcal{E}_{BC} \tag{103}
\end{aligned}$$

$$\begin{aligned}
& \sum_{CA} \frac{1}{\mu_{ABCD}} \left[\left(\frac{V_{BCDM}^A}{A_{BCD}^2} + \frac{V_{ABDM}^C}{A_{ABD}^2} \right) \mathcal{E}_{BD} - \frac{V_{BCDM}^A}{A_{BCD}^2} \cdot \mathcal{E}_{CD} - \right. \\
& \left. - \frac{V_{BCDM}^A}{A_{BCD}^2} \cdot \mathcal{E}_{BC} - \frac{V_{ABDM}^C}{A_{ABD}^2} \cdot \mathcal{E}_{AD} + \frac{V_{ABDM}^C}{A_{ABD}^2} \cdot \mathcal{E}_{AB} \right]
\end{aligned}$$

$$= \omega^2 \left[\sum_{CA} \varepsilon_{ABCD} \cdot \frac{V_{BDSM}^{CA} + V_{BDSM}^{AC}}{l_{BD}^2} \right] \mathcal{E}_{BD} \quad (104)$$

$$\begin{aligned} & \sum_{AB} \frac{o}{\mu_{ABCD}} \left[\left(\frac{V_{ACDM}^B}{A_{ACD}^2} + \frac{V_{BCDM}^A}{A_{BCD}^2} \right) \mathcal{E}_{CD} - \frac{V_{ACDM}^B}{A_{ACD}^2} \cdot \mathcal{E}_{AD} + \right. \\ & \left. + \frac{V_{ACDM}^B}{A_{ACD}^2} \cdot \mathcal{E}_{AC} - \frac{V_{BCDM}^A}{A_{BCD}^2} \cdot \mathcal{E}_{BD} + \frac{V_{BCDM}^A}{A_{BCD}^2} \cdot \mathcal{E}_{BC} \right] \\ & = \omega^2 \left[\sum_{AB} \varepsilon_{ABCD} \cdot \frac{V_{CDSM}^{AB} + V_{CDSM}^{BA}}{l_{CD}^2} \right] \mathcal{E}_{CD} \cdot o \end{aligned} \quad (105)$$

From these equations, the respective proportions of the tetrahedron $ABCD$ for the coefficient matrix M can be ascertained.

(Each equation is set up for an inner edge of the grid and corresponds thus to a line of the matrix M .)

If A_{XYZ}^2 is replaced by \mathbf{A}_{XYZ}^2 and l_{XY}^2 by \mathbf{p}_{XY}^2 , then these proportions are dependent on known quantities alone; for the entries in the main diagonals of M , the following can be derived:

$$i = k(A, B)$$

$$m_{ii} = \frac{1}{\mu_{ABCD}} \left(\frac{V_{ABCM}^D}{\mathbf{A}_{ABC}^2} + \frac{V_{ABDM}^C}{\mathbf{A}_{ABD}^2} \right) - \omega^2 \cdot \varepsilon_{ABCD} \cdot \frac{V_{ABSM}^{CD} + V_{ABSM}^{DC}}{\mathbf{p}_{AB}^2} \quad (106)$$

$$i = k(A, C)$$

$$m_{ii} = \frac{1}{\mu_{ABCD}} \left(\frac{V_{ACDM}^B}{\mathbf{A}_{ACD}^2} + \frac{V_{ABCM}^D}{\mathbf{A}_{ABC}^2} \right) - \omega^2 \cdot \varepsilon_{ABCD} \cdot \frac{V_{ACSM}^{DB} + V_{ACSM}^{BD}}{\mathbf{p}_{AC}^2} \quad (107)$$

$$i = k(A, D)$$

$$m_{ii} = \frac{1}{\mu_{ABCD}} \left(\frac{V_{ABDM}^C}{\mathbf{A}_{ABD}^2} + \frac{V_{ACDM}^B}{\mathbf{A}_{ACD}^2} \right) - \omega^2 \cdot \varepsilon_{ABCD} \cdot \frac{V_{ADSM}^{BC} + V_{ADSM}^{CB}}{\mathbf{p}_{AD}^2} \quad (108)$$

$$i = k(B, C)$$

$$m_{ii} = \frac{1}{\mu_{ABCD}} \left(\frac{V_{ABCM}^D}{\mathbf{A}_{ABC}^2} + \frac{V_{BCDM}^A}{\mathbf{A}_{BCD}^2} \right) - \omega^2 \cdot \varepsilon_{ABCD} \cdot \frac{V_{BCSM}^{AD} + V_{BCSM}^{DA}}{\mathbf{p}_{BC}^2} \quad (109)$$

$$i = k(B, D)$$

$$m_{ii} = \frac{1}{\mu_{ABCD}} \left(\frac{V_{BCDM}^A}{\mathbf{A}_{BCD}^2} + \frac{V_{ABDM}^C}{\mathbf{A}_{ABD}^2} \right) - \omega^2 \cdot \varepsilon_{ABCD} \cdot \frac{V_{BDSM}^{CA} + V_{BDSM}^{AC}}{\mathbf{p}_{BD}^2} \quad (110)$$

Finally, by considering left and right tetrahedra, we have

$$i = k(C, D)$$

$$m_{ii} = \frac{1}{\mu_{ABCD}} \left(\frac{V_{ACDM}^B}{\mathbf{A}_{ACD}^2} + \frac{V_{BCDM}^A}{\mathbf{A}_{BCD}^2} \right) - \omega^2 \cdot \varepsilon_{ABCD} \cdot \frac{V_{CDSM}^{AB} + V_{CDSM}^{BA}}{\mathbf{p}_{CD}^2} \quad (111)$$

For non-diagonal entries, we obtain:

$$i = k(A, B) \quad j = k(B, C) \quad m_{ij} = + \frac{1}{\mu_{ABCD}} \frac{V_{ABCM}^D}{\mathbf{A}_{ABC}^2} \quad (112)$$

$$j = k(A, C) \quad m_{ij} = - \frac{1}{\mu_{ABCD}} \frac{V_{ABCM}^D}{\mathbf{A}_{ABC}^2} \quad (113)$$

$$j = k(B, D) \quad m_{ij} = + \frac{1}{\mu_{ABCD}} \frac{V_{ABDM}^C}{\mathbf{A}_{ABD}^2} \quad (114)$$

$$j = k(A, D) \quad m_{ij} = - \frac{1}{\mu_{ABCD}} \frac{V_{ABDM}^C}{\mathbf{A}_{ABD}^2} \quad (115)$$

$$i = k(A, C) \quad j = k(C, D) \quad m_{ij} = + \frac{1}{\mu_{ABCD}} \frac{V_{ACDM}^B}{\mathbf{A}_{ACD}^2} \cdot o \quad (116)$$

$$j = k(A, D) \quad m_{ij} = - \frac{1}{\mu_{ABCD}} \frac{V_{ACDM}^B}{\mathbf{A}_{ACD}^2} \quad (117)$$

$$j = k(B, C) \quad m_{ij} = - \frac{1}{\mu_{ABCD}} \frac{V_{ABCM}^D}{\mathbf{A}_{ABC}^2} \quad (118)$$

$$j = k(A, B) \quad m_{ij} = - \frac{1}{\mu_{ABCD}} \frac{V_{ABCM}^D}{\mathbf{A}_{ABC}^2} \quad (119)$$

$$i = k(A, D) \quad j = k(B, D) \quad m_{ij} = -\frac{1}{\mu_{ABCD}} \frac{V_{ABDM}^C}{\mathbf{A}_{ABD}^2} \quad (120)$$

$$j = k(A, B) \quad m_{ij} = -\frac{1}{\mu_{ABCD}} \frac{V_{ABDM}^C}{\mathbf{A}_{ABD}^2} \quad (121)$$

$$j = k(C, D) \quad m_{ij} = -\frac{1}{\mu_{ABCD}} \frac{V_{ACDM}^B}{\mathbf{A}_{ACD}^2} \cdot o \quad (122)$$

$$j = k(A, C) \quad m_{ij} = -\frac{1}{\mu_{ABCD}} \frac{V_{ACDM}^B}{\mathbf{A}_{ACD}^2} \quad (123)$$

$$i = k(B, C) \quad j = k(A, C) \quad m_{ij} = -\frac{1}{\mu_{ABCD}} \frac{V_{ABCM}^D}{\mathbf{A}_{ABC}^2} \quad (124)$$

$$j = k(A, B) \quad m_{ij} = +\frac{1}{\mu_{ABCD}} \frac{V_{ABCM}^D}{\mathbf{A}_{ABC}^2} \quad (125)$$

$$j = k(C, D) \quad m_{ij} = +\frac{1}{\mu_{ABCD}} \frac{V_{BCDM}^A}{\mathbf{A}_{BCD}^2} \cdot o \quad (126)$$

$$j = k(B, D) \quad m_{ij} = -\frac{1}{\mu_{ABCD}} \frac{V_{BCDM}^A}{\mathbf{A}_{BCD}^2} \quad (127)$$

$$i = k(B, D) \quad j = k(C, D) \quad m_{ij} = -\frac{1}{\mu_{ABCD}} \frac{V_{BCDM}^A}{\mathbf{A}_{BCD}^2} \cdot o \quad (128)$$

$$j = k(B, C) \quad m_{ij} = -\frac{1}{\mu_{ABCD}} \frac{V_{BCDM}^A}{\mathbf{A}_{BCD}^2} \quad (129)$$

$$j = k(A, D) \quad m_{ij} = -\frac{1}{\mu_{ABCD}} \frac{V_{ABDM}^C}{\mathbf{A}_{ABD}^2} \quad (130)$$

$$j = k(A, B) \quad m_{ij} = +\frac{1}{\mu_{ABCD}} \frac{V_{ABDM}^C}{\mathbf{A}_{ABD}^2} \quad (131)$$

$$i = k(C, D) \quad j = k(A, D) \quad m_{ij} = -\frac{1}{\mu_{ABCD}} \frac{V_{ACDM}^B}{\mathbf{A}_{ACD}^2} \cdot o \quad (132)$$

$$j = k(A, C) \quad m_{ij} = +\frac{1}{\mu_{ABCD}} \frac{V_{ACDM}^B}{\mathbf{A}_{ACD}^2} \cdot o \quad (133)$$

$$j = k(B, D) \quad m_{ij} = -\frac{1}{\mu_{ABCD}} \frac{V_{BCDM}^A}{\mathbf{A}_{BCD}^2} \cdot o \quad (134)$$

$$j = k(B, C) \quad m_{ij} = +\frac{1}{\mu_{ABCD}} \frac{V_{BCDM}^A}{\mathbf{A}_{BCD}^2} \cdot o \quad (135)$$

16 Further simplifications

For the above non-diagonal entries of the coefficient matrix (112) - (135) only four different values occur (up to the sign), namely

$$Q_A = \frac{1}{\mu_{ABCD}} \frac{V_{BCDM}^A}{\mathbf{A}_{BCD}^2} \quad (136)$$

$$Q_B = \frac{1}{\mu_{ABCD}} \frac{V_{ACDM}^B}{\mathbf{A}_{ACD}^2} \quad (137)$$

$$Q_C = \frac{1}{\mu_{ABCD}} \frac{V_{ABDM}^C}{\mathbf{A}_{ABD}^2} \quad (138)$$

$$Q_D = \frac{1}{\mu_{ABCD}} \frac{V_{ABCM}^D}{\mathbf{A}_{ABC}^2} \quad (139)$$

If we further set

$$R_{AB} = \omega^2 \cdot \varepsilon_{ABCD} \cdot \frac{V_{ABSM}^{CD} + V_{ABSM}^{DC}}{\mathbf{p}_{AB}^2} \quad (140)$$

$$R_{AC} = \omega^2 \cdot \varepsilon_{ABCD} \cdot \frac{V_{ACSM}^{DB} + V_{ACSM}^{BD}}{\mathbf{p}_{AC}^2} \quad (141)$$

$$R_{AD} = \omega^2 \cdot \varepsilon_{ABCD} \cdot \frac{V_{ADSM}^{BC} + V_{ADSM}^{CB}}{\mathbf{p}_{AD}^2} \quad (142)$$

$$R_{BC} = \omega^2 \cdot \varepsilon_{ABCD} \cdot \frac{V_{BCSM}^{AD} + V_{BCSM}^{DA}}{\mathbf{p}_{BC}^2} \quad (143)$$

$$R_{BD} = \omega^2 \cdot \varepsilon_{ABCD} \cdot \frac{V_{BDSM}^{CA} + V_{BDSM}^{AC}}{\mathbf{p}_{BD}^2} \quad (144)$$

$$R_{CD} = \omega^2 \cdot \varepsilon_{ABCD} \cdot \frac{V_{CDSM}^{AB} + V_{CDSM}^{BA}}{\mathbf{p}_{CD}^2} \quad (145)$$

we have the following expressions for the diagonal entries of M :

$$i = k(A, B) \quad m_{ii} = Q_C + Q_D - R_{AB} \quad (146)$$

$$i = k(A, C) \quad m_{ii} = Q_B + Q_D - R_{AC} \quad (147)$$

$$i = k(A, D) \quad m_{ii} = Q_B + Q_C - R_{AD} \quad (148)$$

$$i = k(B, C) \quad m_{ii} = Q_A + Q_D - R_{BC} \quad (149)$$

$$i = k(B, D) \quad m_{ii} = Q_A + Q_C - R_{BD} \quad (150)$$

and, by considering right and left tetrahedra,

$$i = k(C, D) \quad m_{ii} = Q_A + Q_B - R_{CD} \quad (151)$$

For the non-diagonal entries, we have

$$i = k(A, B) \quad j = k(B, C) \quad m_{ij} = +Q_D \quad (152)$$

$$j = k(A, C) \quad m_{ij} = -Q_D \quad (153)$$

$$j = k(B, D) \quad m_{ij} = +Q_C \quad (154)$$

$$j = k(A, D) \quad m_{ij} = -Q_C \quad (155)$$

$$i = k(A, C) \quad j = k(C, D) \quad m_{ij} = +Q_B \cdot o \quad (156)$$

$$j = k(A, D) \quad m_{ij} = -Q_B \quad (157)$$

$$j = k(B, C) \quad m_{ij} = -Q_D \quad (158)$$

$$j = k(A, B) \quad m_{ij} = -Q_D \quad (159)$$

$$i = k(A, D) \quad j = k(B, D) \quad m_{ij} = -Q_C \quad (160)$$

$$j = k(A, B) \quad m_{ij} = -Q_C \quad (161)$$

$$j = k(C, D) \quad m_{ij} = -Q_B \cdot o \quad (162)$$

$$j = k(A, C) \quad m_{ij} = -Q_B \quad (163)$$

$$i = k(B, C) \quad j = k(A, C) \quad m_{ij} = -Q_D \quad (164)$$

$$j = k(A, B) \quad m_{ij} = +Q_D \quad (165)$$

$$j = k(C, D) \quad m_{ij} = +Q_A \cdot o \quad (166)$$

$$j = k(B, D) \quad m_{ij} = -Q_A \quad (167)$$

$$i = k(B, D) \quad j = k(C, D) \quad m_{ij} = -Q_A \cdot o \quad (168)$$

$$j = k(B, C) \quad m_{ij} = -Q_A \quad (169)$$

$$j = k(A, D) \quad m_{ij} = -Q_C \quad (170)$$

$$j = k(A, B) \quad m_{ij} = +Q_C \quad (171)$$

$$i = k(C, D) \quad j = k(A, D) \quad m_{ij} = -Q_B \cdot o \quad (172)$$

$$j = k(A, C) \quad m_{ij} = +Q_B \cdot o \quad (173)$$

$$j = k(B, D) \quad m_{ij} = -Q_A \cdot o \quad (174)$$

$$j = k(B, C) \quad m_{ij} = +Q_A \cdot o \quad (175)$$

The remaining six entries of the matrix M , belonging to this tetrahedron, have the value zero:

$$i = k(A, B) \quad j = k(C, D) \quad m_{ij} = m_{ji} = 0 \quad (176)$$

$$i = k(A, C) \quad j = k(B, D) \quad m_{ij} = m_{ji} = 0 \quad (177)$$

$$i = k(A, D) \quad j = k(B, C) \quad m_{ij} = m_{ji} = 0 \quad (178)$$

17 Symmetry of the coefficient matrix

From Section 16 above, it follows that

$$m_{ij} = m_{ji} \quad (179)$$

for each entry in M , belonging to a tetrahedron $ABCD$, whose edges are all inner edges.

Since the first index of m_{ij} always belongs to an inner edge, this equation does not apply, if the second index belongs to the outside edge the entry m_{ji} does not exist, in this case (there is no equation for the outside edges).

If K_i denotes the number of inner edges, then:

$$AB \text{ is inner edge:} \quad k(A, B) \leq K_i \quad (180)$$

$$AB \text{ is outside edge:} \quad k(A, B) > K_i \quad (181)$$

Now for tetrahedra with at least one inner edge (there can be tetrahedra, which possess only outside edges) all entries m_{ij} in the matrix M can be calculated. Here $i \leq K_i$ always applies.

If j belongs to an inner edge, then likewise $j \leq K_i$ applies, and the entry m_{ji} exists. Since $m_{ij} = m_{ji}$, the first $K_i \times K_i$ block of the matrix M is symmetrical.

If j belongs to the outside edge, then $j > K_i$ applies and the entry m_{ji} does not exist. The entry m_{ij} is outside of the first K_i columns of M .

The columns of the matrix M for which $j > K_i$, belong to the outside edges and thus relate to the boundary conditions of the problem.

The actual coefficient matrix for the calculation of the modified electrical field strengths on the edges (multiplied by the length consists of the first K_i columns of M , is square and from the above considerations, symmetric.

18 Demands on the grid generator

In order to generate a tetrahedral grid, in which all the circumcentres of the tetrahedra lie within the respective tetrahedra, and for which any connecting line (Voronoi edge) of two circumcentres of neighbouring tetrahedra lead to no further tetrahedra, two conditions must be fulfilled:

1. No surface is an blunt-angled triangle.
2. The smallest ball around a surface does not contain further nodes.

19 Calculation of the coefficient matrix over the inner surfaces

In Section 15 we calculated the coefficient matrix by regarding all tetrahedra in sequence.

It can also be calculated by regarding all inner surfaces in sequence.

If ABC is an inner surface of the grid, then it is a common surface of two neighbouring tetrahedra. The peaks of these tetrahedra are D_1 and D_2 .

To each combination of two edges of the surface ABC , whereby the first of the edges should be an inner edge of the grid, we compute the corresponding entry in the coefficient matrix, as follows:

$$|m_{ij}| = Q_{D_1} + Q_{D_2} = \frac{1}{\mu_{ABCD_1}} \frac{V_{ABCM}^{D_1}}{\mathbf{A}_{ABC}^2} + \frac{1}{\mu_{ABCD_2}} \frac{V_{ABCM}^{D_2}}{\mathbf{A}_{ABC}^2} \quad (182)$$

Thus

$$|m_{ij}| = \frac{1}{\mathbf{A}_{ABC}^2} \left[\frac{V_{ABCM}^{D_1}}{\mu_{ABCD_1}} + \frac{V_{ABCM}^{D_2}}{\mu_{ABCD_2}} \right] \quad (183)$$

and for the same material in both tetrahedra

$$|m_{ij}| = \frac{V_{ABCM}^{D_1} + V_{ABCM}^{D_2}}{\mu_{ABCD_1} \cdot \mathbf{A}_{ABC}^2} \quad (184)$$

The sign of m_{ij} is determined by edge orientation, based on the direction from smaller to the larger node number.

The following outline shows, the various possible combinations of edge orientations, and the corresponding signs in each case:



fig.7: Sign of the coefficient according to edge orientation

20 Matrix representation

The first two Maxwell equations can be represented (after multiplication with μ_0) as follows:

$$\tilde{\mathbf{C}}\mathbf{D}_{\tilde{s}/\tilde{\mu}}\mathbf{B}_i = j\omega\mu_0\varepsilon_0\mathbf{D}_{\tilde{A}\tilde{\varepsilon}}\mathbf{E}_i \quad (185)$$

$$\mathbf{C}\mathbf{D}_s\mathbf{E} = -j\omega\mathbf{D}_A\mathbf{B}_i \quad (186)$$

Here, we have:

\mathbf{E}	vector of the electrical field strengths on all edges
\mathbf{E}_i	vector of the electrical field strengths on all inner edges
\mathbf{B}_i	vector of the magnetic induction on the inner surfaces
\mathbf{C}	discrete operator of the line integral of the second Maxwell equation
$\tilde{\mathbf{C}}$	discrete operator of the line integral of the first Maxwell equation
\mathbf{D}_s	diagonal matrix of the edge lengths
\mathbf{D}_A	diagonal matrix of the tetrahedron surfaces
$\mathbf{D}_{\tilde{s}/\tilde{\mu}}$	diagonal matrix of the (length proportion/material size) values of the Voronoi edges
$\mathbf{D}_{\tilde{A}\tilde{\varepsilon}}$	diagonal matrix of the (surface portion*material size) values of the Voronoi surfaces

From these equations, we first write

$$-j\omega\tilde{\mathbf{C}}\mathbf{D}_{\tilde{s}/\tilde{\mu}}\mathbf{B}_i = \omega^2\mu_0\varepsilon_0\mathbf{D}_{\tilde{A}\tilde{\varepsilon}}\mathbf{E}_i \quad (187)$$

$$-j\omega\mathbf{B}_i = \mathbf{D}_A^{-1}\mathbf{C}\mathbf{D}_s\mathbf{E}, \quad (188)$$

and then eliminate the \mathbf{B}_i , to get

$$\tilde{\mathbf{C}}\mathbf{D}_{\tilde{s}/\tilde{\mu}}\mathbf{D}_A^{-1}\mathbf{C}\mathbf{D}_s\mathbf{E} = \omega^2\mu_0\varepsilon_0\mathbf{D}_{\tilde{A}\tilde{\varepsilon}}\mathbf{E}_i. \quad (189)$$

With

$$k_0^2 = \omega^2\mu_0\varepsilon_0 \quad (190)$$

we can further write

$$\tilde{\mathbf{C}}\mathbf{D}_{\tilde{s}/\tilde{\mu}}\mathbf{D}_A^{-1}\mathbf{C}\mathbf{D}_s\mathbf{E} - k_0^2\mathbf{D}_{\tilde{A}\tilde{\varepsilon}}\mathbf{E}_i = 0 \quad (191)$$

Since the boundary values on the outside edges are given, the matrices $\mathbf{C}, \mathbf{D}_s, \mathbf{E}$, which belong to the first term of the equation, can be split into two parts: one for the outside edges ($\tilde{\mathbf{C}}, \tilde{\mathbf{D}}_s, \mathbf{E}_a$) and one for the inner edges ($\hat{\mathbf{C}}, \hat{\mathbf{D}}_s, \mathbf{E}_i$).

The known values are now moved to the right-hand side:

$$\tilde{\mathbf{C}}\mathbf{D}_{\tilde{s}/\tilde{\mu}}\mathbf{D}_A^{-1}\hat{\mathbf{C}}\hat{\mathbf{D}}_s\mathbf{E}_i - k_0^2\mathbf{D}_{\tilde{A}\tilde{\varepsilon}}\mathbf{E}_i = -\tilde{\mathbf{C}}\mathbf{D}_{\tilde{s}/\tilde{\mu}}\mathbf{D}_A^{-1}\tilde{\mathbf{C}}\tilde{\mathbf{D}}_s\mathbf{E}_a \quad (192)$$

Here again, we have introduced new notation:

\mathbf{E}_a	vector of the electrical field strengths on the outside edges (boundary values)
$\tilde{\mathbf{C}}$	proportion of \mathbf{C} for the outside edges
$\tilde{\mathbf{D}}_s$	proportion of \mathbf{D}_s for the outside edges
$\hat{\mathbf{C}}$	proportion of \mathbf{C} for the inner edges
$\hat{\mathbf{D}}_s$	proportion of \mathbf{D}_s for the inner edges

Now the equation can be expressed as

$$\left(\tilde{\mathbf{C}} \mathbf{D}_{\tilde{s}/\tilde{\mu}} \mathbf{D}_A^{-1} \hat{\mathbf{C}} - k_0^2 \mathbf{D}_{\tilde{A}\tilde{\epsilon}} \hat{\mathbf{D}}_s^{-1} \right) \left(\hat{\mathbf{D}}_s \mathbf{E}_i \right) = -\tilde{\mathbf{C}} \mathbf{D}_{\tilde{s}/\tilde{\mu}} \mathbf{D}_A^{-1} \tilde{\mathbf{C}} \tilde{\mathbf{D}}_s \mathbf{E}_a \quad (193)$$

The product $\hat{\mathbf{D}}_s \mathbf{E}_i$ corresponds to the variable \mathcal{E} . The symmetry of the first bracketed term has been proven in the Section 17 and we also note that:

$$\hat{\mathbf{C}}^T = \tilde{\mathbf{C}} \quad (194)$$

The order of magnitude of the matrix entries in the first bracketed term roughly amounts to length/surface, thus 1/length. The term remains symmetrical after pre- and post-multiplication by the same diagonal matrix. If the diagonal matrix is based on the square roots of the lengths, then the resulting matrix has entries of $O(1)$. This is achieved by pre-multiplying equation (193) by $\hat{\mathbf{D}}_s^{1/2}$:

$$\hat{\mathbf{D}}_s^{1/2} \tilde{\mathbf{C}} \mathbf{D}_{\tilde{s}/\tilde{\mu}} \mathbf{D}_A^{-1} \hat{\mathbf{C}} \hat{\mathbf{D}}_s \mathbf{E}_i - k_0^2 \hat{\mathbf{D}}_s^{1/2} \mathbf{D}_{\tilde{A}\tilde{\epsilon}} \mathbf{E}_i = -\hat{\mathbf{D}}_s^{1/2} \tilde{\mathbf{C}} \mathbf{D}_{\tilde{s}/\tilde{\mu}} \mathbf{D}_A^{-1} \tilde{\mathbf{C}} \tilde{\mathbf{D}}_s \mathbf{E}_a \quad (195)$$

or

$$\left(\hat{\mathbf{D}}_s^{1/2} \tilde{\mathbf{C}} \mathbf{D}_{\tilde{s}/\tilde{\mu}} \mathbf{D}_A^{-1} \hat{\mathbf{C}} \hat{\mathbf{D}}_s^{1/2} - k_0^2 \mathbf{D}_{\tilde{A}\tilde{\epsilon}} \right) \left(\hat{\mathbf{D}}_s^{1/2} \mathbf{E}_i \right) = -\hat{\mathbf{D}}_s^{1/2} \tilde{\mathbf{C}} \mathbf{D}_{\tilde{s}/\tilde{\mu}} \mathbf{D}_A^{-1} \tilde{\mathbf{C}} \tilde{\mathbf{D}}_s \mathbf{E}_a \quad (196)$$

The quantity $\hat{\mathbf{D}}_s^{1/2} \mathbf{E}_i$ is taken as a new variable. The first bracketed term is then a symmetrical coefficient matrix.

This equation is the basis for the program *efm*.

The third Maxwell equation can be expressed in the form

$$\tilde{\mathbf{S}}_i \mathbf{D}_{\tilde{A}\tilde{\epsilon}} \mathbf{E}_i = 0 \quad (197)$$

The divergence at an internal node is obtained by dividing this equation by the volume of the appropriate Voronoi cell, i.e.

$$\text{div}(\varepsilon \mathbf{E}) = \hat{\mathbf{D}}_V^{-1} \tilde{\mathbf{S}}_i \mathbf{D}_{\tilde{A}\tilde{\epsilon}} \mathbf{E}_i = 0 \quad (198)$$

Here, we have:

$\tilde{\mathbf{S}}_i$ discrete divergence operator on the binary grid for the inner nodes
 $\hat{\mathbf{D}}_{\tilde{V}}$ diagonal matrix of the volumes of the Voronoi - cells around internal nodes

where

$$\left(\tilde{\mathbf{S}}_i\right)_{ij} = \begin{cases} 1 & \text{if edge } j \text{ is directed away from node } i \\ -1 & \text{if edge } j \text{ is directed towards node } i \\ 0 & \text{otherwise} \end{cases} \quad (199)$$

applies.

For the normal derivative component, we have

$$\mathbf{n} \cdot \text{grad } U = \frac{\partial U(\mathbf{r})}{\partial \mathbf{n}} = \lim_{\Delta t \rightarrow 0} \frac{U(\mathbf{r} + \Delta t \mathbf{n}) - U(\mathbf{r})}{\Delta t} \quad (200)$$

For an edge from node i to node j , we have in the discrete case:

$$\text{grad } U \cdot \mathbf{n}_{ij} = \frac{U_j - U_i}{l_{ij}} \quad (201)$$

For all inner edges it thereby follows that

$$\text{grad } U \cdot \mathbf{n} = -\hat{\mathbf{D}}_s^{-1} \mathbf{S} \mathbf{U} \quad (202)$$

with:

\mathbf{S} discrete gradients of the edge directions
 \mathbf{U} amount of a scalar field in all nodes

and where

$$\mathbf{S}_{ij} = \begin{cases} 1 & \text{if edge } i \text{ is directed away from node } j \\ -1 & \text{if edge } i \text{ is directed towards node } j \\ 0 & \text{otherwise} \end{cases} \quad (203)$$

applies.

For the outer nodes, $\text{div}(\varepsilon \mathbf{E}) = 0$, but no Voronoi cells exist. We set

$$\text{div}(\varepsilon \mathbf{E}) = \mathbf{D}_{\tilde{V}}^{-1} \tilde{\mathbf{S}} \mathbf{D}_{\tilde{A}\tilde{\varepsilon}} \mathbf{E}_i \quad (204)$$

where

$\mathbf{D}_{\tilde{V}}^{-1}$ modification to $\hat{\mathbf{D}}_{\tilde{V}}$, by setting a zero into the main diagonal
on the place of outside edges
 $\tilde{\mathbf{S}}$ extension of $\tilde{\mathbf{S}}_i$ on the outside edges according to the condition for \mathbf{S}_{ij}

Setting $U = \text{div}(\varepsilon \mathbf{E})$, we get

$$\text{graddiv}(\varepsilon \mathbf{E}) \cdot \mathbf{n} = -\hat{\mathbf{D}}_s^{-1} \mathbf{S} \mathbf{D}_{\tilde{V}}^{-1} \tilde{\mathbf{S}} \mathbf{D}_{\tilde{A}\tilde{\varepsilon}} \mathbf{E}_i = 0 \quad (205)$$

From the definitions of \mathbf{S} and $\tilde{\mathbf{S}}$ it follows immediately that

$$\mathbf{S}^T = \tilde{\mathbf{S}}. \quad (206)$$

To similarly obtain a symmetrical coefficient matrix with entries of $O(1)$, from equation (205), we pre-multiply this two diagonal matrices:

$$-\hat{\mathbf{D}}_s^{1/2} \mathbf{D}_{\tilde{A}\tilde{\varepsilon}} \hat{\mathbf{D}}_s^{-1} \mathbf{S} \mathbf{D}_{\tilde{V}}^{-1} \tilde{\mathbf{S}} \mathbf{D}_{\tilde{A}\tilde{\varepsilon}} \mathbf{E}_i = 0, \quad (207)$$

i.e.

$$\left(-\hat{\mathbf{D}}_s^{-1/2} \mathbf{D}_{\tilde{A}\tilde{\varepsilon}} \mathbf{S} \mathbf{D}_{\tilde{V}}^{-1} \tilde{\mathbf{S}} \mathbf{D}_{\tilde{A}\tilde{\varepsilon}} \hat{\mathbf{D}}_s^{-1/2} \right) \left(\hat{\mathbf{D}}_s^{1/2} \mathbf{E}_i \right) = 0 \quad (208)$$

It is favourable, to express the equation independently of ε , i.e. to regions considers with only one material. This can be achieved, not by dividing by the volumes of the Voronoi - cells, but by dividing by the multiples of the volumes proportionately and by the square of the appropriate ε :

$$\left(-\hat{\mathbf{D}}_s^{-1/2} \mathbf{D}_{\tilde{A}\tilde{\varepsilon}} \mathbf{S} \mathbf{D}_{\tilde{V}\tilde{\varepsilon}\tilde{\varepsilon}}^{-1} \tilde{\mathbf{S}} \mathbf{D}_{\tilde{A}\tilde{\varepsilon}} \hat{\mathbf{D}}_s^{-1/2} \right) \left(\hat{\mathbf{D}}_s^{1/2} \mathbf{E}_i \right) = 0 \quad (209)$$

$\mathbf{D}_{\tilde{V}\tilde{\varepsilon}\tilde{\varepsilon}}^{-1}$ similarly to $\mathbf{D}_{\tilde{V}}^{-1}$, volume proportions are multiplied by ε^2

Equation (209) possesses a symmetrical coefficient matrix and likewise the variable $\hat{\mathbf{D}}_s^{1/2} \mathbf{E}_i$; in the program *efm* it is used for preconditioning.

21 Documentation for the program efm

1. General

With the program **efm** (electric field matrix), we assemble the coefficient matrix on the right-hand side of a set of linear equations for the calculation of an electric field on a tetrahedral grid.

The starting point is an input file, which consists of the geometrical sizes of the tetrahedral grid, the material sizes, the considered frequency and the values at the gates, which are calculated from an eigenvalue problem.

In order that the developing coefficient matrix remains symmetric, the variables of the electrical field strengths on edges are multiplied by the roots of the respective edge lengths.

Apart from the log file, the formatted and the unformatted files of the set of equations (coefficient matrix and right-hand side) and some further files, used for checking purposes, the remainder are output files.

2. The input file

The input file **datei** contains no keywords and no separating blank lines. Real and complex numbers are inputted with double precision.

The fundamental structure is:

```
frequency  
material  
nodes  
x y z  
tetrahedra  
n1 n2 n3 n4 mat  
outside edges      boundary values  
n1 n2 E0
```

By frequency, we mean here the rotational frequency $\omega = ak_0 \cdot c$.

Under material firstly the number of different materials is indicated, then all relative values μ (real) and finally all relative values ε (complex).

Following the entry for the number of nodes, the x, y, z coordinates are written, line by line.

The number of tetrahedra comes next, followed by a 5-number set for each tetrahedron; the first four numbers are the node numbers of the corner nodes and the fifth number indicates the material of the tetrahedron.

Finally, the number of the outside edges and the number of the boundary values are

written. Among these, in each case, are the starting node and the end node and the boundary value belonging to this edge, which can only be non-zero at the gates. The outside edges require a boundary value, so that the set of equations becomes uniquely solvable. Further boundary values can be obtained by noting that all edges of the electrical conductor take the boundary value zero. (If the electrical conductor is not discretised, but is regarded as a hole, then only the appropriate outside edges are to be set zero).

3. The program **efm**

The program **efm** is written in FORTRAN90. After starting the program with „efm“, the input file **datei** is selected and afterwards the output files for the coefficient matrix **datei1** and the right-hand side **datei2**, as well as the type of output, either as a file or as files IA, JA and AA for the coefficients matrix.

Further, the preconditioner *graddiv* may be selected (or not), and the minimum values (MinVoro, MinVol) for the Voronoi surface and the volume of a tetrahedron are selected.

The program first reads in the input values.

There is no internal check, to see whether the tetrahedral grid satisfies the Delaunay criterion.

Circumcentres of circumspheres located outside of the given tetrahedron are considered within the calculation.

The different stages of the program can be followed interactively.

These are written also into a log file, which carries the same name as the input file and carries the suffix „.prt“.

4. The output files

datei.prt : This file includes information to the given minimum values, the details barring date and time of day of the calculation, whether or not *graddiv* was implemented and the names of the input and output files. Also some information concerning the tetrahedral grid and the set of equations, along with the computing times required for reading the input file, for the calculation and for the output in files; the edge numbers, the entry numbers and the values for the maximum and the minimum entries (absolute values) of the right-hand side (b) and the coefficient matrix (A).

IAdatei1.fmt, JAdatei1.fmt, AAdatei1.fmt, datei1.fmt : Formatted output of the coefficient matrix.

Since the coefficient matrix is symmetric, only the right upper triangular part is stored here.

Since the matrix is sparse, it is stored in the form IA, JA, AA. These are three lists or column vectors with only one entry for each line. If *dim* is the dimension of the matrix and *eintr* the number of non-zero entries (NNE) in the matrix, then the length of the list IA is $dim + 1$ and of the lists JA and AA is *eintr*.

In the list IA the number of the first NNE of the i th line of the matrix is located in the i th line. In the $(dim + 1)$ th line is the increased (by an amount 1) number of the NNE of the matrix.

The column numbers of the NNE are located in the list JA, while the NNE itself are found in the list AA.

The lists IA, JA and AA are stored in the files **IAdatei1.fmt**, **JAdatei1.fmt** and **AAdatei1.fmt** or in the separate file **datei1.fmt**, where in the latter case, first the dimension of the matrix and then the lists IA,JA,AA are stored.

IAdatei1.unf, **JAdatei1.unf**, **AAdatei1.unf**, **datei1.unf** : Appropriate unformatted output of the coefficient matrix

datei2.fmt : Formatted output of the right-hand sides of the equations

datei2.unf : Unformatted output of the right-hand sides of the equations

vanish : File of the edges with disappearing Voronoi surfaces.

During the generation of grid edges, it is possible that the circumcentres of the circumferences of the surrounding tetrahedra can collapse to one point, i.e. the Voronoi surface can disappear. In the coefficient matrix, only zeros are located in the appropriate line and the field strength on the edges cannot be calculated. So that the set of equations remains solvable, a „1“ is inserted on the main diagonal, whereby the electrical field strength on this edge acquires a (false) value of zero.

In the file, the edge numbers are stored line by line from start to end node.

edges : The edge list KantList($i,1:2$) is stored as a two-dimensional field for the index i .

If *Nodes* is the number of the nodes and *Edges* the number of edges of the grid ($Edges = dim$), then the index i runs from $-Nodes$ to *Edges*.

Each edge is determined by its start and end node, whereby the end node has a larger node number than the starting node.

A is the node number of any node. Kantlist (-A,1) indicates the number of edges with the starting node A. If this value is non-zero, then KantList (-A,2) shows a positive index. This index is the edge number of the edge with the starting node A and the end node KantL ($i1,1$). If there are further edges with the starting node A, then KantList ($i1,2$) points to the next edging number, etc.. For the last edge with starting node A, the index 0 is shown.

edgenodes : In this file, the edges are stored with their start and end nodes.

length : In this file, the edge lengths are stored.

sqrtl : In this file, the square roots of the edge lengths are stored. After solving the set of equations, we can get the electric field strengths on grid edges by dividing the solution by these square roots.

22 A small example

As an example we have simulated a rectangular microwave structure. The structure is subdivided in $3 \times 3 \times 2$ equidistant rectangular three-dimensional elementary cells. The two cells in the middle of the structure are the electrical conductor. Furthermore every rectangular elementary cell is subdivided in six tetrahedra.

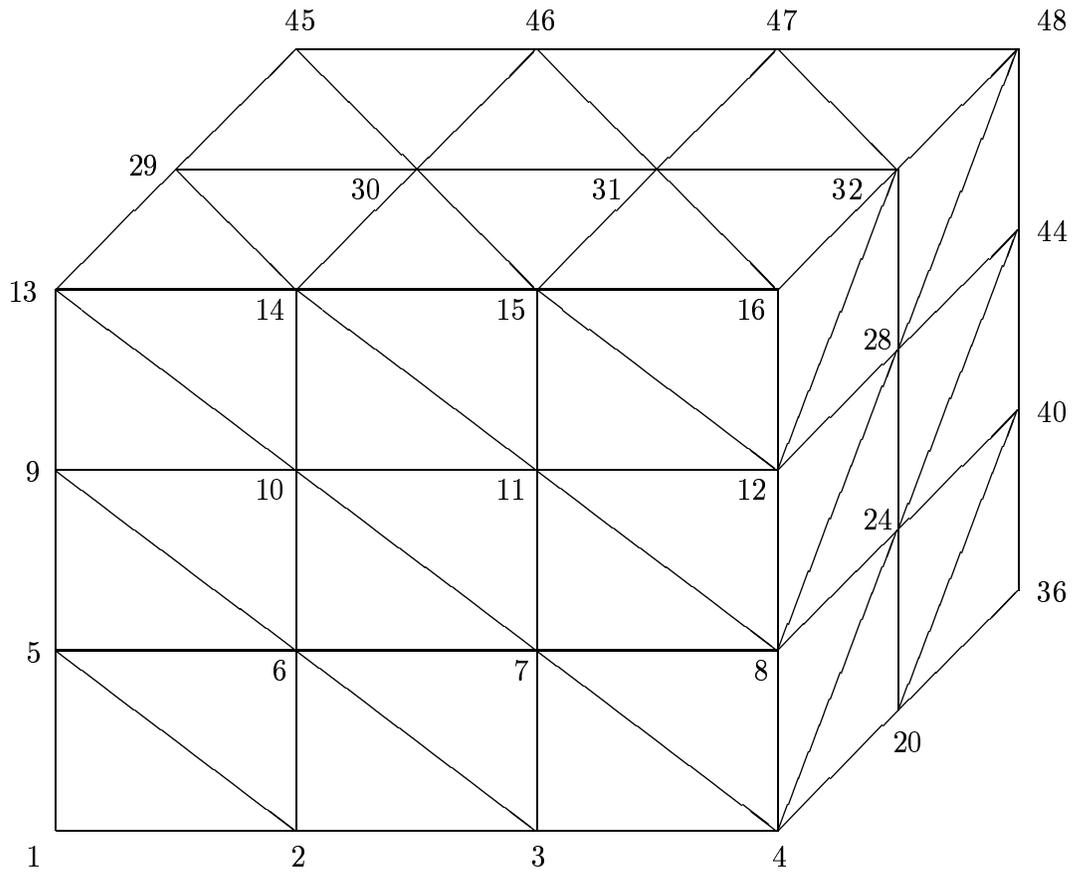


fig.8: The subdivided structure

The material constants of the electrical conductor do not influence the computation, because all edges of the conductor take the boundary value zero. The only gate is in front of the structure. The other sides are electric walls. One get the following input file:

599584916.D0
 2
 1.0D0
 1.0D0
 (1.0D0,-0.1D0)
 (1.0D0,0.0D0)
 48
 0.0000000000000000D+000 0.0000000000000000D+000 0.0000000000000000D+000
 4.0000000000000000D-001 0.0000000000000000D+000 0.0000000000000000D+000
 8.0000000000000000D-001 0.0000000000000000D+000 0.0000000000000000D+000
 1.2000000000000000D+000 0.0000000000000000D+000 0.0000000000000000D+000
 0.0000000000000000D+000 0.0000000000000000D+000 3.0000000000000000D-001
 4.0000000000000000D-001 0.0000000000000000D+000 3.0000000000000000D-001
 ...
 0.0000000000000000D+000 0.0000000000000000D+000 6.0000000000000000D-001
 ...
 0.0000000000000000D+000 0.0000000000000000D+000 9.0000000000000000D-001
 ...
 0.0000000000000000D+000 2.5000000000000000D-001 0.0000000000000000D+000
 4.0000000000000000D-001 2.5000000000000000D-001 0.0000000000000000D+000
 ...
 0.0000000000000000D+000 2.5000000000000000D-001 3.0000000000000000D-001
 ...
 1.2000000000000000D+000 5.0000000000000000D-001 9.0000000000000000D-001
 108
 1 5 2 21 1
 5 6 2 21 1
 6 22 2 21 1
 22 18 2 21 1
 18 17 2 21 1
 17 1 2 21 1
 2 6 3 22 1
 ...
 27 31 28 47 1
 31 32 28 47 1
 32 48 28 47 1
 48 44 28 47 1
 44 43 28 47 1
 43 27 28 47 1
 126 149
 1 5 0.0D0
 2 6 (8.2100000000000000D-001,4.1090000000000000D-002)
 3 7 (8.2100000000000000D-001,4.1090000000000000D-002)
 4 8 0.0D0
 5 9 0.0D0

6 10 0.0D0
7 11 0.0D0
8 12 0.0D0
9 13 0.0D0
10 14 (8.210000000000000D-001,4.109000000000000D-002)
11 15 (8.210000000000000D-001,4.109000000000000D-002)
12 16 0.0D0
33 37 0.0D0
...
1 2 0.0D0
2 3 0.0D0
3 4 0.0D0
5 6 (1.134000000000000D+000,4.692000000000000D-001)
6 7 0.0D0
7 8 (1.134000000000000D+000,4.692000000000000D-001)
9 10 (1.134000000000000D+000,4.692000000000000D-001)
10 11 0.0D0
11 12 (1.134000000000000D+000,4.692000000000000D-001)
13 14 0.0D0
14 15 0.0D0
15 16 0.0D0
...
1 17 0.0D0
17 33 0.0D0
2 18 0.0D0
...
2 5 (-2.073000000000000D-001,-1.753530000000000D-001)
3 6 (4.926000000000000D-001,2.465400000000000D-002)
4 7 (-2.073000000000000D-001,-1.753530000000000D-001)
6 9 (9.072000000000000D-001,3.753600000000000D-001)
7 10 0.0D0
8 11 (9.072000000000000D-001,3.753600000000000D-001)
10 13 (-2.073000000000000D-001,-1.753530000000000D-001)
11 14 (4.926000000000000D-001,2.465400000000000D-002)
12 15 (-2.073000000000000D-001,-1.753530000000000D-001)
34 37 0.0D0
...
1 21 0.0D0
17 37 0.0D0
...
2 17 0.0D0
3 18 0.0D0
4 19 0.0D0
...
6 22 0.0D0

```

22 38 0.0D0
7 23 0.0D0
...
22 23 0.0D0
26 27 0.0D0
22 26 0.0D0
23 27 0.0D0
23 26 0.0D0
6 26 0.0D0
...
7 22 0.0D0
...
7 26 0.0D0
23 42 0.0D0

```

There are 197 variables, but 149 variables are boundary values.

After the computation there are 16 variables in the file **vanish**. These variables belong to the diagonals of the rectangular cells (without the two rectangular cells of the electrical conductor), because the circumcentres of the circumspheres of the surrounding tetrahedra collapse to one point, i.e. the Voronoi surfaces disappear. The belonging edges are stored from start to end node.

2	21
3	22
4	23
6	25
8	27
10	29
11	30
12	31
18	37
19	38
20	39
22	41
24	43
26	45
27	46
28	47

In the resulting matrix there are 231 entries.

The structure was computed for the tetrahedral grid on the one hand and for rectangular cells on the other hand. The values on the edges of the rectangular cells do not differ in the two cases.

23 Conclusions

The test calculations showed that good results can be achieved with the program **efm** on tetrahedron grids and that by the use of **graddiv** as preconditioner, a faster convergence is attained.

Further tests and investigations are useful in order to find criteria (dependent on the grid) for the parameters **MinVoro**, **MinVol** and **Minzei**, which on the one hand should serve to prevent unreasonably small entries in the matrix, but on the other hand can also set relevant entries to zero.

A further step would be to integrate the various components, ranging from the grid generator to the calculation of the scattering matrix, into a large program.

24 Nomenclature

\mathbf{A}_{ABC}	inwardly-arranged surface vector of the triangle ABC
A_{ABC}	surface of the triangle ABC
\mathbf{B}_i	vector of the magnetic induction on the inner surfaces
$\mathbf{B}(S_{ABC})$	magnetic induction (vector) in S_{ABC}
B_{ABC}	real or complex number (magnetic induction)
\mathbf{C}	discrete operator of the line integral of the second Maxwell equation
$\tilde{\mathbf{C}}$	discrete operator of the line integral of the first Maxwell equation
$\hat{\mathbf{C}}$	proportion of \mathbf{C} for the inner edges
$\check{\mathbf{C}}$	proportion of \mathbf{C} for the outside edges
\mathbf{D}_A	diagonal matrix of the tetrahedron surfaces
$\mathbf{D}_{\tilde{A}\tilde{\epsilon}}$	diagonal matrix of the (surface portion*material size) values of the Voronoi surfaces
\mathbf{D}_s	diagonal matrix of the edge lengths
$\mathbf{D}_{\tilde{s}/\tilde{\mu}}$	diagonal matrix of the (length proportion/material size) values of the Voronoi edges
$\mathbf{D}_{\tilde{V}}$	modification to $\hat{\mathbf{D}}_{\tilde{V}}$, by setting a zero into the main diagonal on the place of outside edges
$\mathbf{D}_{\tilde{V}\tilde{\epsilon}\tilde{\epsilon}}$	similarly to $\mathbf{D}_{\tilde{V}}$, volume proportions are multiplied by ϵ^2
$\hat{\mathbf{D}}_s$	proportion of \mathbf{D}_s for the inner edges
$\check{\mathbf{D}}_s$	proportion of \mathbf{D}_s for the outside edges
$\hat{\mathbf{D}}_{\tilde{V}}$	diagonal matrix of the volumes of the Voronoi - cells around internal nodes
d_{AB}^C	distance of the circumcenter of the triangle ABC to the side AB
\mathbf{E}	vector of the electrical field strengths on all edges
\mathbf{E}_a	vector of the electrical field strengths on the outside edges (boundary values)
\mathbf{E}_i	vector of the electrical field strengths on all inner edges
$\mathbf{E}(S_{AB})$	electrical field strength (vector) in S_{AB}
E	number of nodes
E_0	number of nodes of the surface network
E_A	nodes of the polyhedron around node A
E_{AB}	real or complex number (electrical field strength)
E_i	number of internal nodes
\mathcal{E}	variable vector of the electrical field
\mathcal{E}_{AB}	modified electrical field strength on the edge AB
\mathcal{E}_i	variable of the electrical field
F	number of surfaces
F_0	number of surfaces of the surface network
F_i	number of internal surfaces (nodes, edges may be situated outside)
F_i	the side opposite node \mathbf{p}_i
\mathbf{g}_i	surface vector of F_i directed towards the inside of the tetrahedron divided by the threefold volume of the tetrahedron
h_i	height of the point \mathbf{p}_i over F_i

K	number of edges
K_0	number of edges of the surface network
$k(A, B)$	index assigned to the edge AB
K_i	number of internal edges (nodes may be situated outside)
l_{AB}	length of side AB
l_{ABC}^D	distance of the circumcentre of the tetrahedron $ABCD$ to the side ABC
M	circumcentre of the sphere
M	coefficient matrix
M_{ABCD}	circumcentre of the tetrahedron $ABCD$
m_{ij}	coefficient matrix entry
N	number of nodes
\mathbf{n}_{AB}	unit vector in AB direction
\mathbf{n}_{ABC}	normal vector, which is perpendicular to the triangle ABC , (with a mathematically positive arrangement of the nodes A, B, C)
\mathbf{n}_i	normal to F_i , which is belonging directed away from the tetrahedron interior
\mathbf{p}_A	vector to the node A
$P_K(\cdot)$	projection onto the appropriate edge
$P_N(\cdot)$	projection onto the appropriate surface-normal
Q_A	simplification of an entry in M
R	radius of the sphere
R_{AB}	simplification of an entry in the main diagonal of M
\mathbf{S}	discrete gradients of the edge directions
S_{AB}	center of the edge AB
S_{ABC}	circumcentre of the triangle ABC
\mathbf{S}_{ABC}	vector for the circumcentre of the triangle ABC
$\tilde{\mathbf{S}}$	extension of $\tilde{\mathbf{S}}_i$ on the outside edges according to the condition for \mathbf{S}_{ij}
$\tilde{\mathbf{S}}_i$	discrete divergence operator on the binary grid for the inner nodes
SP	double product of the vectors (lowest node first)
T	number of tetrahedra
\mathbf{U}	amount of a scalar field in all nodes
V_A	volume of the Voronoi cell around the node A
V_{ABCD}	volume of the tetrahedron $ABCD$
V_{ABCM}^D	volume of the tetrahedron $ABCM$, whereby M is the circumcentre of the tetrahedron $ABCD$
V_{ABSM}^{CD}	Volume of the tetrahedron $ABSM$, whereby M is the circumcentre of the tetrahedron $ABCD$ and S is the circumcenter of the surface ABC
x_A	x component of the vector \mathbf{p}_A
y_A	y component of the vector \mathbf{p}_A
z_A	z component of the vector \mathbf{p}_A
$\varepsilon_{ABCD}, \mu_{ABCD}$	material constants in the tetrahedron $ABCD$
ω	rotational frequency

References

- [1] Beilenhoff, K., Heinrich, W., Hartnagel, H. L. (1992): Improved Finite-Difference Formulation in Frequency Domain for Three-Dimensional Scattering Problems. *IEEE Transactions on Microwave Theory and Techniques*, **40**, 540-546
- [2] Christ, A., Hartnagel, H. L. (1987): Three-Dimensional Finite-Difference Method for the Analysis of Microwave-Device Embedding, *IEEE Transactions on Microwave Theory and Techniques*, **35**, No. 8, 688-696
- [3] Hebermehl, G., Schlundt, R., Zscheile, H., Heinrich W. (1999): Improved Numerical Methods for the Simulation of Microwave Circuits, *Surveys on Mathematics for Industry*, **9**, No. 2, 117-129
- [4] Tischler, T., Heinrich, W. (2000): The Perfectly Matched Layer as Lateral Boundary in Finite-Difference Transmission-Line Analysis. *2000 Int. Microwave Symp. Digest* **1**, 121-124
- [5] Hebermehl, G., Hübner, F.-K., Schlundt, R., Tischler, T., Zscheile, H., Heinrich W. (2001): On the Computation of Eigen Modes for Lossy Microwave Transmission Lines Including Perfectly Matched Layer Boundary Conditions, *The International Journal for Computation and Mathematics in Electrical and Electronic Engineering*, **20**, No. 4, 948-964
- [6] Hebermehl, G., Hübner, F.-K., Schlundt, R., Tischler, T., Zscheile, H., Heinrich W. (2001): Numerical Simulation of Lossy Microwave Transmission Lines Including PML, In: van Rienen, U., Günther, M., Hecht, D. (ed.) *Lecture Notes in Computational Science and Engineering, Scientific Computing in Electrical Engineering*, **18**, 267-275
- [7] Schlundt, R., Hebermehl, G., Hübner, F.-K., Tischler, T., Zscheile, H., Heinrich W. (2001): Iterative Solution of Systems of Linear Equations in Microwave Circuits Using a Block Quasi-Minimal Residual Algorithm, In: van Rienen, U., Günther, M., Hecht, D. (ed.) *Lecture Notes in Computational Science and Engineering, Scientific Computing in Electrical Engineering*, **18**, 325-333
- [8] Fuhrmann, J., Langmach, H., Schmelzer, I. (2001): pdelib, <http://www.wias-berlin.de/pdelib/doc/index.html>
- [9] Schmelzer, I. (2000): Grid Generation and Geometry Description with COG, in *Proceedings of contributed papers and posters, ALGORITHM 2000, 15th Conference on Scientific Computing, Vysoké Tatry - Podbanské, Slovakia, September 10 - 15, 2000*, Ed. A. Handlovičová, M. Kormorníková, K. Mikula, D. Ševčovič, Slovak University of Technology, Bratislava, 399-405
- [10] Schmelzer, I. (2000): COG, <http://www.wias-berlin.de/cog/index.html>

- [11] George, P.-L., Borouchaki, H. (1998): Delaunay Triangulation and Meshing, Editions Hermes, Paris
- [12] Uhle, M., (1999): LBG - Layer Based Grid Generator, <http://www.wias-berlin.de/pdelib/doc/lbg.html-dir/index.html>
- [13] Fuhrmann, J., Langmach, H., Schmelzer, I., Uhle, M. (1999): Grid Management in pdelib, <http://www.wias-berlin.de/pdelib/doc/index.html>, sxgrid.ps, 1–29
- [14] Eisenstat, S. C.: Efficient implementation of a class of preconditioned conjugate gradient methods. SIAM J. Sci Statist. Comput. **2** (1981) 1–4
- [15] Freund, R. W., Malhotra, W.: A Block-QMR Algorithm for Non-Hermitian Linear Systems with Multiple Right-Hand Sides. Linear Algebra and Its Applications, **254** (1997) 119–157
- [16] Saad, Y.: Iterative methods for sparse linear systems. PWS Publishing Company (1996)

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