Resistor Models for Diffusion in 3-D

Introduction

Almost any Finite Element book starts with the assembly of resistor-like finite elements, without approximations (if you consider Ohm's law as being "exact"). Contained in [1] is a chapter about "Electrical Networks". The matrix of an electrical resistor is derived *directly*, by applying the laws of Ohm and Kirchhoff, giving:

$$\begin{bmatrix} +1/R & -1/R \\ -1/R & +1/R \end{bmatrix}$$

where R are the resistances. Defining admittances A instead of resistances R turns out to be more convenient in this context, the relationship between the two being simply $A = 1/R$. The finite element matrix of a resistor is then given by:

$$\begin{bmatrix} +A & -A \\ -A & +A \end{bmatrix}$$

Further define the connectivity (no coordinates!) of the resistor-network, and apply two voltages. The standard FE assembly procedure can be carried out then in a straightforward manner.

Linear Tetrahedron

Let's consider the simplest non-trivial finite element shape in 3-D, which is a *linear tetrahedron*. Function behaviour is approximated inside such a tetrahedron by a *linear* interpolation between the function values at the vertices, also called nodal points. Let T be such a function, and x, y, z coordinates, then:

$$T = A.x + B.y + C.z + D$$

Where the constants A, B, C, D are yet to be determined. Substitute $x = x_k$, $y = y_k$, $z = z_k$ with $k = 0, 1, 2, 3$. Start with:

$$T_0 = A.x_0 + B.y_0 + C.z_0 + D$$

Clearly, the first of these equations can already be used to eliminate the constant D, once and forever:

$$T - T_0 = A.(x - x_0) + B.(y - y_0) + C.(z - z_0)$$

Then the constants A , B , C are determined by:

$$\begin{aligned} T_1 - T_0 &= A.(x_1 - x_0) + B.(y_1 - y_0) + C.(z_1 - z_0) \\ T_2 - T_0 &= A.(x_2 - x_0) + B.(y_2 - y_0) + C.(z_2 - z_0) \\ T_3 - T_0 &= A.(x_3 - x_0) + B.(y_3 - y_0) + C.(z_3 - z_0) \end{aligned}$$

Three equations with three unknowns. A solution can be found:

$$\begin{bmatrix} A \\ B \\ C \end{bmatrix} = \begin{bmatrix} x_1 - x_0 & y_1 - y_0 & z_1 - z_0 \\ x_2 - x_0 & y_2 - y_0 & z_2 - z_0 \\ x_3 - x_0 & y_3 - y_0 & z_3 - z_0 \end{bmatrix}^{-1} \begin{bmatrix} T_1 - T_0 \\ T_2 - T_0 \\ T_3 - T_0 \end{bmatrix}$$

It is concluded that A, B, C and hence $(T - T_0)$ must be a linear expression in the $(T_k - T_0)$:

$$\begin{aligned} T - T_0 &= \xi.(T_1 - T_0) + \eta.(T_2 - T_0) + \zeta.(T_3 - T_0) \\ &= \begin{bmatrix} \xi & \eta & \zeta \end{bmatrix} \begin{bmatrix} T_1 - T_0 \\ T_2 - T_0 \\ T_3 - T_0 \end{bmatrix} \end{aligned}$$

See above:

$$= \begin{bmatrix} \xi & \eta & \zeta \end{bmatrix} \begin{bmatrix} x_1 - x_0 & y_1 - y_0 & z_1 - z_0 \\ x_2 - x_0 & y_2 - y_0 & z_2 - z_0 \\ x_3 - x_0 & y_3 - y_0 & z_3 - z_0 \end{bmatrix} \begin{bmatrix} A \\ B \\ C \end{bmatrix}$$

See above:

$$= T - T_0 = \begin{bmatrix} x - x_0 & y - y_0 & z - z_0 \end{bmatrix} \begin{bmatrix} A \\ B \\ C \end{bmatrix}$$

Hence:

$$\begin{aligned} x - x_0 &= \xi.(x_1 - x_0) + \eta.(x_2 - x_0) + \zeta.(x_3 - x_0) \\ y - y_0 &= \xi.(y_1 - y_0) + \eta.(y_2 - y_0) + \zeta.(y_3 - y_0) \\ z - z_0 &= \xi.(z_1 - z_0) + \eta.(z_2 - z_0) + \zeta.(z_3 - z_0) \end{aligned}$$

But also:

$$T - T_0 = \xi.(T_1 - T_0) + \eta.(T_2 - T_0) + \zeta.(T_3 - T_0)$$

Therefore the *same* expression holds for the function T as well as for the coordinates x, y, z. This is called an *isoparametric* transformation. It is remarked without proof that the *local coordinates* ξ, η, ζ within a tetrahedron can be interpreted as sub-volumes, spanned by the vectors $\vec{r}_k - \vec{r}_0$ and $\vec{r} - \vec{r}_0$ where $\vec{r} = (x, y, z)$ and $k = 1, 2, 3$.
Reconsider the expression:

$$T - T_0 = \xi.(T_1 - T_0) + \eta.(T_2 - T_0) + \zeta.(T_3 - T_0)$$

Partial differentiation to ξ , η , ζ gives:

$$\partial T/\partial \xi = T_1 - T_0 \quad ; \quad \partial T/\partial \eta = T_2 - T_0 \quad ; \quad \partial T/\partial \zeta = T_3 - T_0$$

Therefore:

$$T = T(0) + \xi \frac{\partial T}{\partial \xi} + \eta \frac{\partial T}{\partial \eta} + \zeta \frac{\partial T}{\partial \zeta}$$

This is part of a Taylor series expansion around node (0). Such Taylor series expansions are very common in Finite Difference analysis. Now rewrite as follows:

$$T = (1 - \xi - \eta - \zeta).T_0 + \xi.T_1 + \eta.T_2 + \zeta.T_3$$

Here the functions $(1-\xi-\eta-\zeta), \xi, \eta, \zeta$ are called the *shape functions* of a Finite Element. Shape functions N_k have the property that they are unity in one of the nodes (k), and zero in all other nodes. In our case:

$$N_0 = 1 - \xi - \eta - \zeta \quad ; \quad N_1 = \xi \quad ; \quad N_2 = \eta \quad ; \quad N_3 = \zeta$$

So we have two representations, which are allmost trivially equivalent:

$$\begin{array}{ll} T = T_0 + \xi.(T_1 - T_0) + \eta.(T_2 - T_0) + \zeta.(T_3 - T_0) & : \text{Finite Difference} \\ T = (1 - \xi - \eta - \zeta).T_0 + \xi.T_1 + \eta.T_2 + \zeta.T_3 & : \text{Finite Element} \end{array}$$

What kind of terms can be discretized at the domain of a linear tetrahedron? In the first place, the function $T(x, y, z)$ itself, of course. But one may also try on the first order partial derivatives $\partial T/\partial(x, y, z)$. We find:

$$\partial T/\partial x = A \quad ; \quad \partial T/\partial y = B \quad ; \quad \partial T/\partial z = C$$

Using the expressions which were found for A, B, C:

$$\begin{bmatrix} \partial T/\partial x \\ \partial T/\partial y \\ \partial T/\partial z \end{bmatrix} = \begin{bmatrix} x_1 - x_0 & y_1 - y_0 & z_1 - z_0 \\ x_2 - x_0 & y_2 - y_0 & z_2 - z_0 \\ x_3 - x_0 & y_3 - y_0 & z_3 - z_0 \end{bmatrix}^{-1} \begin{bmatrix} T_1 - T_0 \\ T_2 - T_0 \\ T_3 - T_0 \end{bmatrix}$$

It is seen from this formula that one must determine the inverse of the above matrix first. This can be done with Cramer's rule, as follows:

```
      subroutine dinv3(mat,det)
*                =====
*     Direct inversion of 3 x 3 matrix
*     --------------------------------
      real mat(3,3),sub(3,3)
*
      sub(1,1)=+mat(2,2)*mat(3,3)-mat(2,3)*mat(3,2)
      sub(2,1)=-mat(1,2)*mat(3,3)+mat(1,3)*mat(3,2)
      sub(3,1)=+mat(1,2)*mat(2,3)-mat(1,3)*mat(2,2)
*
      sub(1,2)=-mat(2,1)*mat(3,3)+mat(2,3)*mat(3,1)
      sub(2,2)=+mat(1,1)*mat(3,3)-mat(1,3)*mat(3,1)
      sub(3,2)=-mat(1,1)*mat(2,3)+mat(1,3)*mat(2,1)
*
      sub(1,3)=+mat(2,1)*mat(3,2)-mat(2,2)*mat(3,1)
      sub(2,3)=-mat(1,1)*mat(3,2)+mat(1,2)*mat(3,1)
      sub(3,3)=+mat(1,1)*mat(2,2)-mat(1,2)*mat(2,1)
*
      det=mat(1,1)*mat(2,2)*mat(3,3)-mat(1,1)*mat(2,3)*mat(3,2)
     +   -mat(2,1)*mat(1,2)*mat(3,3)+mat(2,1)*mat(1,3)*mat(3,2)
     +   +mat(3,1)*mat(1,2)*mat(2,3)-mat(3,1)*mat(1,3)*mat(2,2)
*
      if(det.eq.0.) stop 'dinv3: det=0'
*
      do 10 i=1,3
      do 10 j=1,3
10    mat(i,j)=sub(j,i)/det
*
      return
      end
```

While carrying out this algorithm, terms can be rewritten as in:

$$(x_1 - x_0)(y_2 - y_0) - (x_2 - x_0)(y_1 - y_0) =$$

$$= x_1y_2 + x_2y_0 + x_0y_1 - x_2y_1 - x_0y_2 - x_1y_0 = \begin{vmatrix} 1 & x_0 & y_0 \\ 1 & x_1 & y_1 \\ 1 & x_2 & y_2 \end{vmatrix}$$

The following shorthand notation will be used for all this:

$$(x, y; 0, 1, 2) = \begin{vmatrix} 1 & x_0 & y_0 \\ 1 & x_1 & y_1 \\ 1 & x_2 & y_2 \end{vmatrix}$$

Let's do the real thing now. Inverting the above matrix then results in:

$$\begin{bmatrix} \partial T/\partial x \\ \partial T/\partial y \\ \partial T/\partial z \end{bmatrix} = \begin{bmatrix} (y,z;2,3,0) & (y,z;3,0,1) & (y,z;0,1,2) \\ (z,x;2,3,0) & (z,x;3,0,1) & (z,x;0,1,2) \\ (x,y;2,3,0) & (x,y;3,0,1) & (x,y;0,1,2) \end{bmatrix} /\Delta \begin{bmatrix} T_1 - T_0 \\ T_2 - T_0 \\ T_3 - T_0 \end{bmatrix}$$

Here Δ is the determinant of the original matrix as a whole. In order to find the coefficients belonging to T_0, add up the columns of the inverted matrix and provide the sum with a minus sign:

$$-\begin{bmatrix} (y,z;2,3,0)+(y,z;3,0,1)+(y,z;0,1,2) \\ (z,x;2,3,0)+(z,x;3,0,1)+(z,x;0,1,2) \\ (x,y;2,3,0)+(x,y;3,0,1)+(x,y;0,1,2) \end{bmatrix} T_0 = \begin{bmatrix} (y,z;1,2,3) \\ (z,x;1,2,3) \\ (x,y;1,2,3) \end{bmatrix} T_0$$

The righthand side being the result of a little exercise in elementary algebra. We have found a 3×4 *Differentiation Matrix*, which represents the gradient operator $\partial/\partial(x,y,z)$ for the function values $T_{0,1,2,3}$ at a linear tetrahedron:

$$\begin{bmatrix} \partial/\partial x \\ \partial/\partial y \\ \partial/\partial z \end{bmatrix} = \begin{bmatrix} (y,z;1,2,3) & (y,z;2,3,0) & (y,z;3,0,1) & (y,z;0,1,2) \\ (z,x;1,2,3) & (z,x;2,3,0) & (z,x;3,0,1) & (z,x;0,1,2) \\ (x,y;1,2,3) & (x,y;2,3,0) & (x,y;3,0,1) & (x,y;0,1,2) \end{bmatrix} /\Delta$$

It is seen that each column of the differentiation matrix corresponds with a component of the normal (cross product) belonging to the area of the triangle opposite to the vertex where the accompanying temperature is defined, thereby everything being divided by the volume of the tetrahedron as a whole.

This for example means that the gradient of the temperature field is described in a sensible way as a flux through all triangle boundaries of the tetrahedron.

The above procedure of finding the differentiation matrix entries for T_0 thus means that the normal on triangle $(1,2,3)$ is equal to minus the sum of the normals on the other triangles. Which in turn means that the (vector) sum of all normals is equal to zero, which indeed should be the case for any *closed* (tetrahedal) surface.

Discretization for 3-D Diffusion

Consider the three-dimensional Laplace-like term, which is defined in Cartesian coordinates by:

$$\frac{\partial Q_x}{\partial x} + \frac{\partial Q_y}{\partial y} + \frac{\partial Q_z}{\partial z}$$

where:

$$\begin{bmatrix} Q_x \\ Q_y \\ Q_z \end{bmatrix} = \begin{bmatrix} \partial T/\partial x \\ \partial T/\partial y \\ \partial T/\partial z \end{bmatrix}$$

Here T = temperature, x, y, z = coordinates. Suppose the contribution is valid in a domain D with boundary S. According to the so called Galerkin method, the contribution is multiplied by an arbitrary function f and then integrated over the Domain of interest. Since the function f is completely arbitrary (well, continuous at least), this is supposed to be equivalent to the original problem:

$$\iiint f(x,y,z)\left(\frac{\partial Q_x}{\partial x}+\frac{\partial Q_y}{\partial y}+\frac{\partial Q_z}{\partial z}\right)dx.dy.dz$$

The advantage of the Galerkin formulation is that we are able now to convert second order derivatives into first order derivatives. To see how this works, let us recall Green's theorem, or partial integration for triple integrals, by which the following expression can be substituted for the Galerkin integral:

$$\oint\!\!\oint f.Q_n\,dS \quad - \quad \iiint\left(Q_x\frac{\partial f}{\partial x}+Q_y\frac{\partial f}{\partial y}+Q_z\frac{\partial f}{\partial z}\right)dx.dy.dz$$

The first of these terms incorporates boundary conditions at the surface S. The boundary integral is *zero* in case the normal derivative $Q_n = 0$. For this reason $Q_n = 0$ is called a *natural* boundary condition: it is fulfilled *automatically* if the first term in the above formulation is simply discarded.

The second term is an integral for the *bulk* material. Substitute temperature fluxes herein and watch out for the minus sign:

$$-\iiint\begin{bmatrix}\frac{\partial f}{\partial x} & \frac{\partial f}{\partial y} & \frac{\partial f}{\partial z}\end{bmatrix}\begin{bmatrix}\partial T/\partial x\\ \partial T/\partial y\\ \partial T/\partial z\end{bmatrix}dx.dy.dz$$

Note that the second order derivatives have been removed indeed. It is possible to handle second order problems with first order (linear) finite elements only.

If the integration domain is subdivided into finite elements E, then the above integral is splitted up as a sum of integrals over these elements. Integration is always carried out numerically, by using *integration points* [2]. A little bit of innovation is involved in recognizing that it doesn't make much difference if the integration points are deliberately chosen in such a way that evaluation is as easy as possible: we always select them at the vertices of any elements involved. It can be shown that elements which are integrated in such a way are in fact *superpositions of linear tetrahedra*. Linear tetrahedra are so to speak the ultimate 3-D elements and there's no need for anything else most of the time. At such linear tetrahedra, differentiations $\partial/\partial(x, y, z)$ are given as a matrix operation, with the *Differentiation Matrices* found in an earlier stage. Here is the symbolic representation for the element-matrix contributions belonging to the diffusion term, using differentiation matrices $\partial/\partial(x, y, z)$:

$$\begin{bmatrix}\partial/\partial x & \partial/\partial y & \partial/\partial z\end{bmatrix}\begin{bmatrix}\partial/\partial x\\ \partial/\partial y\\ \partial/\partial z\end{bmatrix}\Delta$$

Here Δ = determinant (volume) of the tetrahedron. Using the end-result of the preceding chapter:

$$\begin{bmatrix} \partial/\partial x \\ \partial/\partial y \\ \partial/\partial z \end{bmatrix} = \begin{bmatrix} (y,z;1,2,3) & (y,z;2,3,0) & (y,z;3,0,1) & (y,z;0,1,2) \\ (z,x;1,2,3) & (z,x;2,3,0) & (z,x;3,0,1) & (z,x;0,1,2) \\ (x,y;1,2,3) & (x,y;2,3,0) & (x,y;3,0,1) & (x,y;0,1,2) \end{bmatrix} / \Delta$$

Now we are going to use the accompanying interpretation: the columns of the differentiation matrix are components of normals $\vec{N}$ on triangles which are at the boundary of each tetrahedron. Finite element matrices for diffusion can be written down then in the following form, finally:

$$\begin{bmatrix} \vec{N}_{123}\cdot\vec{N}_{123} & \vec{N}_{123}\cdot\vec{N}_{230} & \vec{N}_{123}\cdot\vec{N}_{301} & \vec{N}_{123}\cdot\vec{N}_{012} \\ \vec{N}_{230}\cdot\vec{N}_{123} & \vec{N}_{230}\cdot\vec{N}_{230} & \vec{N}_{230}\cdot\vec{N}_{301} & \vec{N}_{230}\cdot\vec{N}_{012} \\ \vec{N}_{301}\cdot\vec{N}_{123} & \vec{N}_{301}\cdot\vec{N}_{230} & \vec{N}_{301}\cdot\vec{N}_{301} & \vec{N}_{301}\cdot\vec{N}_{012} \\ \vec{N}_{012}\cdot\vec{N}_{123} & \vec{N}_{012}\cdot\vec{N}_{230} & \vec{N}_{012}\cdot\vec{N}_{301} & \vec{N}_{012}\cdot\vec{N}_{012} \end{bmatrix} / \Delta$$

Where it should be mentioned that, in addition:

$$\vec{N}_{123} + \vec{N}_{230} + \vec{N}_{301} + \vec{N}_{012} = 0$$

Hence it's easy to show that each row of the matrix sums up to zero.

If the above result is specialized for a Finite Difference mesh, then the three normals $\vec{N}_{012}$, $\vec{N}_{301}$ and $\vec{N}_{230}$ will be orthogonal to each other. It's a nice exercise to show that the well known F.D. scheme for diffusion can be reconstructed in this case.

Resistor model for 3-D diffusion

Let us devise for example a tetrahedron, built up from electrical resistors. Six (6) of these should be associated with the six sides of the tetrahedron. Let the vertices of the tetrahedron be numbered $0, 1, 2, 3$ and the accompanying admittances be named accordingly. Assemble the accompanying element-matrices:

$$\begin{bmatrix} +A_{01} & -A_{01} & 0 & 0 \\ -A_{01} & +A_{01} & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix} + \begin{bmatrix} +A_{02} & 0 & -A_{02} & 0 \\ 0 & 0 & 0 & 0 \\ -A_{02} & 0 & +A_{02} & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix} + \begin{bmatrix} +A_{03} & 0 & 0 & -A_{03} \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ -A_{03} & 0 & 0 & -A_{03} \end{bmatrix} +$$

$$\begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & +A_{12} & -A_{12} & 0 \\ 0 & -A_{12} & +A_{12} & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix} + \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & +A_{13} & 0 & -A_{13} \\ 0 & 0 & 0 & 0 \\ 0 & -A_{13} & 0 & +A_{13} \end{bmatrix} + \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & +A_{23} & -A_{23} \\ 0 & 0 & -A_{23} & +A_{23} \end{bmatrix}$$

Giving:

$$\begin{bmatrix} A_{01}+A_{02}+A_{03} & -A_{01} & -A_{02} & -A_{03} \\ -A_{01} & A_{01}+A_{12}+A_{13} & -A_{12} & -A_{13} \\ -A_{02} & -A_{12} & A_{02}+A_{12}+A_{23} & -A_{23} \\ -A_{03} & -A_{13} & -A_{23} & A_{03}+A_{13}+A_{23} \end{bmatrix}$$

It is trivially seen that each row of the matrix sums up to zero. Let's compare this with the finite element matrix for 3-D diffusion, as has been found in the preceding paragraph:

$$\begin{bmatrix} \vec{N}_{123}\cdot\vec{N}_{123} & \vec{N}_{123}\cdot\vec{N}_{230} & \vec{N}_{123}\cdot\vec{N}_{301} & \vec{N}_{123}\cdot\vec{N}_{012} \\ \vec{N}_{230}\cdot\vec{N}_{123} & \vec{N}_{230}\cdot\vec{N}_{230} & \vec{N}_{230}\cdot\vec{N}_{301} & \vec{N}_{230}\cdot\vec{N}_{012} \\ \vec{N}_{301}\cdot\vec{N}_{123} & \vec{N}_{301}\cdot\vec{N}_{230} & \vec{N}_{301}\cdot\vec{N}_{301} & \vec{N}_{301}\cdot\vec{N}_{012} \\ \vec{N}_{012}\cdot\vec{N}_{123} & \vec{N}_{012}\cdot\vec{N}_{230} & \vec{N}_{012}\cdot\vec{N}_{301} & \vec{N}_{012}\cdot\vec{N}_{012} \end{bmatrix} / \Delta$$

Now it is possible to identify terms in the diffusion matrix and the resistor matrix respectively:

$$\begin{aligned} A_{01} &= -\vec{N}_{123}\cdot\vec{N}_{230}/\Delta \\ A_{02} &= -\vec{N}_{123}\cdot\vec{N}_{301}/\Delta \\ A_{03} &= -\vec{N}_{123}\cdot\vec{N}_{012}/\Delta \\ A_{12} &= -\vec{N}_{230}\cdot\vec{N}_{301}/\Delta \\ A_{13} &= -\vec{N}_{230}\cdot\vec{N}_{012}/\Delta \\ A_{23} &= -\vec{N}_{301}\cdot\vec{N}_{012}/\Delta \end{aligned}$$

Thus we can consider the 4×4 matrix for diffusion at a tetrahedron as a superposition of one-dimensional resistor-like elements, where any resistor corresponds with the inner product of the normals of the two triangles which are *not* adjacent to the side corresponding with the resistor (divided by the volume of the tetrahedron).

Resistors are positive if (and only if) the corresponding inner products of the normals are negative. This means that the accompanying boundary triangle planes have to make sharp angles which each other.

It is seen that for a (rectangular) Finite Difference grid the normals on the triangles (012),(230) and (301) will be perpendicular to each other and therefore the accompanying inner products will be zero. Hence in this special case: $A_{12} = A_{13} = A_{23} = 0$.

When assembling these element matrices into the global system, most resistors have to be replaced by parallel resistors, one resistor for each side of a tetrahedron, according to the law of superposition. Exceptions are at the boundary.

Bibliography

[1] Norrie D.H. and de Vries G., "An Introduction to Finite Element Analysis", Acad. Press 1978.

[2] O.C. Zienkiewicz, "The Finite Element Method", 3th edition, Mc.Graw-Hill U.K. 1977.