2-D Elementary Substructures

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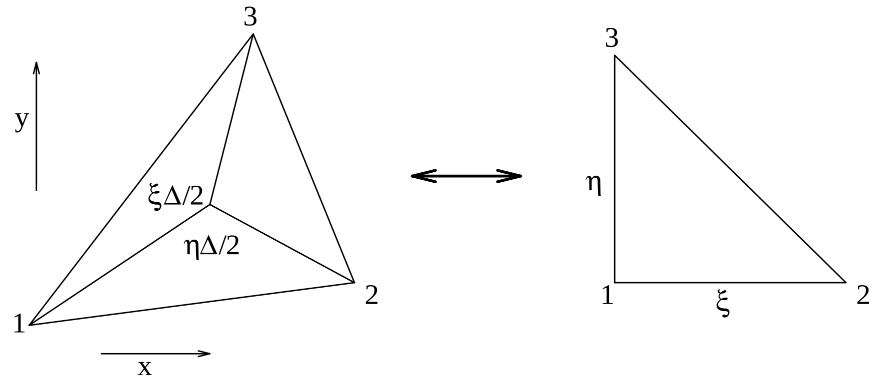
The purpose of this study is to re-establish some definite relationships between Finite Difference and Finite Element Methods. As such, it may be considered as a continuation of my '*Series on Unified Numerical Approximations*' (SUNA). A new result is the generalization of Patankar's F.V. schemes for CONvection *and* difFUSION (also called *confusion*), for meshes consisting of F.E. triangles.

Triangle Algebra

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

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

Where the constants A, B, C are yet to be determined.



Substitute $x = x_k$ and $y = y_k$ with $k = 1, 2, 3$:

$$\begin{bmatrix} T_1 \\ T_2 \\ T_3 \end{bmatrix} = \begin{bmatrix} 1 & x_1 & y_1 \\ 1 & x_2 & y_2 \\ 1 & x_3 & y_3 \end{bmatrix} \begin{bmatrix} C \\ A \\ B \end{bmatrix}$$

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

$$T_1 = A.x_1 + B.y_1 + C$$

Resulting in:

$$T - T_1 = A.(x - x_1) + B.(y - y_1)$$

Hence the constants A and B are determined by:

$$\begin{array}{l} T_2 - T_1 = A.(x_2 - x_1) + B.(y_2 - y_1) \\ T_3 - T_1 = A.(x_3 - x_1) + B.(y_3 - y_1) \end{array}$$

Two equations with two unknowns. The solution is found by straightforward elimination, or by applying Cramer's rule:

$$\begin{array}{l} A = [(y_3 - y_1).(T_2 - T_1) - (y_2 - y_1).(T_3 - T_1)]/\Delta \\ B = [(x_2 - x_1).(T_3 - T_1) - (x_3 - x_1).(T_2 - T_1)]/\Delta \end{array}$$

There are several forms of the determinant Δ, which should be memorized when it is appropriate:

$$\begin{array}{l} \Delta = (x_2 - x_1).(y_3 - y_1) - (x_3 - x_1).(y_2 - y_1) \\ \Delta = 2 \times \text{ area of triangle} \\ \Delta = x_1.y_2 + x_2.y_3 + x_3.y_1 - y_1.x_2 - y_2.x_3 - y_3.x_1 \\ \Delta = x_1.(y_2 - y_3) + x_2.(y_3 - y_1) + x_3.(y_1 - y_2) \\ \Delta = y_1.(x_3 - x_2) + y_2.(x_1 - x_3) + y_3.(x_2 - x_1) \\ \Delta = \left\| \begin{array}{ccc} 1 & x_1 & y_1 \\ 1 & x_2 & y_2 \\ 1 & x_3 & y_3 \end{array} \right\| \end{array}$$

Anyway, it is concluded that:

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

Where:

$$\begin{array}{l} \xi = [(y_3 - y_1).(x - x_1) - (x_3 - x_1).(y - y_1)]/\Delta \\ \eta = [(x_2 - x_1).(y - y_1) - (y_2 - y_1).(x - x_1)]/\Delta \end{array}$$

Or:

$$\left[\begin{array}{c} \xi \\ \eta \end{array} \right] = \left[\begin{array}{cc} +(y_3 - y_1) & -(x_3 - x_1) \\ -(y_2 - y_1) & +(x_2 - x_1) \end{array} \right] /\Delta \left[\begin{array}{c} x - x_1 \\ y - y_1 \end{array} \right]$$

The inverse of the following problem is recognized herein:

$$\left[\begin{array}{c} x - x_1 \\ y - y_1 \end{array} \right] = \left[\begin{array}{cc} (x_2 - x_1) & (x_3 - x_1) \\ (y_2 - y_1) & (y_3 - y_1) \end{array} \right] \left[\begin{array}{c} \xi \\ \eta \end{array} \right]$$

Or:

$$\begin{array}{l} x - x_1 = \xi.(x_2 - x_1) + \eta.(x_3 - x_1) \\ y - y_1 = \xi.(y_2 - y_1) + \eta.(y_3 - y_1) \end{array}$$

But also:

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

Therefore the *same* expression holds for the function T as well as for the coordinates x and y . This is precisely what people mean by an *isoparametric* ("same parameters") transformation, a terminology which is quite common in Finite Element contexts. Now recall the formulas which express ξ and η into x and y :

$$\xi = [(y_3 - y_1).(x - x_1) - (x_3 - x_1).(y - y_1)]/\Delta$$
$$\eta = [(x_2 - x_1).(y - y_1) - (y_2 - y_1).(x - x_1)]/\Delta$$

Thus ξ can be interpreted as: area of the sub-triangle spanned by the vectors $(x-x_1, y-y_1)$ and (x_3-x_1, y_3-y_1) divided by the whole triangle area. And η can be interpreted as: area of the sub-triangle spanned by the vectors $(x-x_1, y-y_1)$ and $(x_2 - x_1, y_2 - y_1)$ divided by the whole triangle area. This is the reason why ξ and η are sometimes called *area-coordinates*; see the above figure, where (two times) the area of the triangle as a whole is denoted as Δ. There exist even *three* of these coordinates in literature. But the third area-coordinate is, of course, dependent on the other two, being equal to $(1 - \xi - \eta)$. Instead of area-coordinates, we prefer to talk about *local coordinates* ξ and η of an element, in contrast to the *global coordinates* x and y. It is possible that local coordinates coincide with the global coordinates. A triangle for which such is the case is called a *parent element*. The portrait of the parent triangle is also depicted in the above figure: it is rectangular, and two sides of it are equal.
Let's reconsider the expression:

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

Partial differentiation to ξ and η gives:

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

Therefore, with node (1) as the origin, hence $T(0) = T_1$:

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

This is part of a Taylor series expansion around node (1). Such Taylor series expansions are quite common in Finite Difference analysis. Now rewrite as follows:

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

Here the functions $(1 - \xi - \eta)$, ξ, η are called the *shape functions* of the 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:

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

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

$$T = T_1 + \xi.(T_2 - T_1) + \eta.(T_3 - T_1) \qquad : \text{Finite Difference like}$$
$$T = (1 - \xi - \eta).T_1 + \xi.T_2 + \eta.T_3 \qquad : \text{Finite Element like}$$

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

$$\partial T/\partial x = A = [(y_3 - y_1).(T_2 - T_1) - (y_2 - y_1).(T_3 - T_1)]/\Delta$$
$$\partial T/\partial y = B = [(x_2 - x_1).(T_3 - T_1) - (x_3 - x_1).(T_2 - T_1)]/\Delta$$

By collecting terms belonging to the same T_k, this can also be written as:

$$\Delta \begin{bmatrix} \partial T/\partial x \\ \partial T/\partial y \end{bmatrix} = \begin{bmatrix} +(y_2 - y_3) & +(y_3 - y_1) & +(y_1 - y_2) \\ -(x_2 - x_3) & -(x_3 - x_1) & -(x_1 - x_2) \end{bmatrix} \begin{bmatrix} T_1 \\ T_2 \\ T_3 \end{bmatrix}$$

Or, in operator form:

$$\begin{bmatrix} \partial/\partial x \\ \partial/\partial y \end{bmatrix} = \begin{bmatrix} y_2 - y_3 & y_3 - y_1 & y_1 - y_2 \\ x_3 - x_2 & x_1 - x_3 & x_2 - x_1 \end{bmatrix} /\Delta$$

The right hand side will be called a *Differentiation Matrix* in subsequent work. Thus the gradient operator at any linear triangle is represented by a 2×3 differentiation matrix.

Conservation of Heat

The Numerical Analysis of Diffusion starts with a well known Partial Differential Equation (PDE). The problem will be restricted *here* to the simpler case of two space dimensions:

$$\frac{\partial Q_x}{\partial x} + \frac{\partial Q_y}{\partial y} = 0$$

(x,y) = Planar coordinates. A possible interpretation of the vector (Q_x, Q_y) is the heat flux. The differential equation then follows from the law of conservation of energy. In case of pure diffusion of heat, also known as conduction, the components of the heat flux are related to temperature as follows:

$$Q_x = -\lambda \frac{\partial T}{\partial x} \qquad Q_y = -\lambda \frac{\partial T}{\partial y}$$

Where λ = thermal conductivity. Hence the final differential equation for the temperature field is actually of the second degree. In order to make the PDE amenable for numerical treatment, an integration procedure has to be resorted to. At this point, there occurs a splitting into several distinct roads, all leading to a numerical solution, more or less efficiently.

When using a Finite Element method, the differential equation is multiplied at first with an arbitrary (test)function. Subsequently the PDE is integrated over the domain of interest. Let the test function be called f, then:

$$\iint f. \left[\frac{\partial Q_x}{\partial x} + \frac{\partial Q_y}{\partial y} \right] dxdy = 0$$

It can be shown that this integral formulation is equivalent with the original partial differential equation. This is due to the fact that f is an *arbitrary* function. It should be continuous and integrable, though.
Partial integration, or applying Green's theorem (which is precisely the same), results in an expression with line-integrals over the boundaries and an area integral over the bulk field. The latter is given by:

$$-\iint \left[\frac{\partial f}{\partial x}.Q_x + \frac{\partial f}{\partial y}.Q_y \right] dxdy$$

Watch the minus sign. The advantage accomplished herewith is a reduction of the difficulty of the problem: only derivatives of the *first* degree are left. As a next step, the domain of interest is split up into "elements" E. Due to this, also the integral will split up into separate contributions, each contribution corresponding with an element:

$$-\sum_E \iint \left[\frac{\partial f}{\partial x}.Q_x + \frac{\partial f}{\partial y}.Q_y \right] dxdy$$

The simplest Finite Element in two dimensions is the linear triangle: read the previous section titled "Triangle Algebra". Essential ingredient of the theory is the so called Differentiation Matrix. Any partial derivative at a linear triangle can be discretized easily with help of such a differentiation matrix:

$$\Delta \begin{bmatrix} \partial f/\partial x \\ \partial f/\partial y \end{bmatrix} = \begin{bmatrix} +(y_2 - y_3) & +(y_3 - y_1) & +(y_1 - y_2) \\ -(x_2 - x_3) & -(x_3 - x_1) & -(x_1 - x_2) \end{bmatrix} \begin{bmatrix} f_1 \\ f_2 \\ f_3 \end{bmatrix}$$

Here Δ is the area of a vector parallelogram, which is twice the area of the triangle. It is clear that $\partial f/\partial x$ and $\partial f/\partial y$ are constants. While considering only 2-D diffusion, Q_x and Q_y are also partial derivatives of the first degree, hence constants. Herewith the bulk Finite Element formulation, for one triangle, is given by:

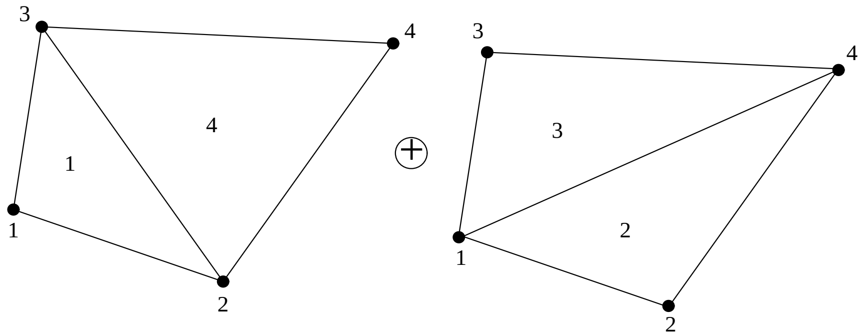
$$-\left[\frac{\partial f}{\partial x}.Q_x + \frac{\partial f}{\partial y}.Q_y \right] \iint dxdy = -\left[\frac{\partial f}{\partial x}.Q_x + \frac{\partial f}{\partial y}.Q_y \right] \Delta/2$$

The remaining integral is equal, namely, to de area of the triangle. Applying now the differentiation matrix, we find:

$$= -\frac{1}{2} \begin{bmatrix} f_1 & f_2 & f_3 \end{bmatrix} \begin{bmatrix} y_2 - y_3 & x_3 - x_2 \\ y_3 - y_1 & x_1 - x_3 \\ y_1 - y_2 & x_2 - x_1 \end{bmatrix} \begin{bmatrix} Q_x \\ Q_y \end{bmatrix} =$$

$$= \frac{1}{2} \begin{bmatrix} f_1 & f_2 & f_3 \end{bmatrix} \begin{bmatrix} (y_3 - y_2)Q_x - (x_3 - x_2)Q_y \\ (y_1 - y_3)Q_x - (x_1 - x_3)Q_y \\ (y_2 - y_1)Q_x - (x_2 - x_1)Q_y \end{bmatrix}$$

Actually, we don't want to subdivide the Finite Element domain into triangular elements, but rather into quadrilateral elements. However, any quad element, in turn, can be subdivided yet into triangles, even in two different ways:



In addition, what we want is a configuration in which all quad vertices play an equally important role. In order to accomplish this, all of the four triangles must be present in our formulation, simultaneously. For just one quadrilateral, it boils down to renumbering vertices in the formulation for a single triangle, according to the following permutations:

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1 2 3        2 4 1        3 1 4        4 3 2
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Also an upper label (*not* a power) will be attached to the values (Q_x, Q_y), because it must be denoted at which triangle the discretization takes place. Any contributions are summed now over the four triangles (and the whole is divided by a factor two again):

$$\frac{1}{4}\begin{bmatrix} f_1 & f_2 & f_3 \end{bmatrix}\begin{bmatrix} (y_3-y_2)Q_x^1-(x_3-x_2)Q_y^1 \\ (y_1-y_3)Q_x^1-(x_1-x_3)Q_y^1 \\ (y_2-y_1)Q_x^1-(x_2-x_1)Q_y^1 \end{bmatrix}+$$

$$\frac{1}{4}\begin{bmatrix} f_2 & f_4 & f_1 \end{bmatrix}\begin{bmatrix} (y_1-y_4)Q_x^2-(x_1-x_4)Q_y^2 \\ (y_2-y_1)Q_x^2-(x_2-x_1)Q_y^2 \\ (y_4-y_2)Q_x^2-(x_4-x_2)Q_y^2 \end{bmatrix}+$$

$$\frac{1}{4}\begin{bmatrix} f_3 & f_1 & f_4 \end{bmatrix}\begin{bmatrix} (y_4-y_1)Q_x^3-(x_4-x_1)Q_y^3 \\ (y_3-y_4)Q_x^3-(x_3-x_4)Q_y^3 \\ (y_1-y_3)Q_x^3-(x_1-x_3)Q_y^3 \end{bmatrix}+$$

$$\frac{1}{4}\begin{bmatrix} f_4 & f_3 & f_2 \end{bmatrix}\begin{bmatrix} (y_2-y_3)Q_x^4-(x_2-x_3)Q_y^4 \\ (y_4-y_2)Q_x^4-(x_4-x_2)Q_y^4 \\ (y_3-y_4)Q_x^4-(x_3-x_4)Q_y^4 \end{bmatrix}$$

Another way to arrive at a formulation in which all four triangles are involved is via Numerical Integration. The implementation of numerical integration is done most efficiently, for quadrilaterals, by choosing four integration points (often called Gauss points) inside the quadrilateral. According to standard theory, these points are located at positions $(\xi,\eta) = 1/(2\sqrt{3})$. (Read the section "Quadrilateral Algebra" for an explanation of ξ and η). It is possible, however, to interpret the exact location of the "Gauss" points with a pinch of salt. The integration points then can be located simply at the vertices (which are only a small distance apart from the "true" locations anyway). Quadrilaterals then behave as if they are composed of overlapping triangles, as depicted in the above figure. It is also clearer now where the weighting factor 1/4 comes from: there are 4 integration points. And quantities Q^k are associated not only with the four triangles, but also with the four vertices of the original quadrilateral.

In order to save unnecessary paperwork, the following shorthand notation has been adopted. It may be interpreted as an outer product:

$$r_{ij} \times Q_k = (y_i - y_j)Q_x^k - (x_i - x_j)Q_y^k = (x_j - x_i)Q_y^k - (y_j - y_i)Q_x^k$$

Terms belonging to $f_k, k = 1...4$ are collected together. By doing so, the standard Finite Element assembly procedure is demonstrated at a small scale. What else is the Finite Element matrix than just an incomplete system of equations?

$$\frac{1}{4}\begin{bmatrix} f_1 & f_2 & f_3 & f_4 \end{bmatrix} \begin{bmatrix} r_{32} \times Q_1 + r_{42} \times Q_2 + r_{34} \times Q_3 + 0 \\ r_{13} \times Q_1 + r_{14} \times Q_2 + 0 + r_{34} \times Q_4 \\ r_{21} \times Q_1 + 0 + r_{41} \times Q_3 + r_{42} \times Q_4 \\ 0 + r_{21} \times Q_2 + r_{13} \times Q_3 + r_{23} \times Q_4 \end{bmatrix}$$

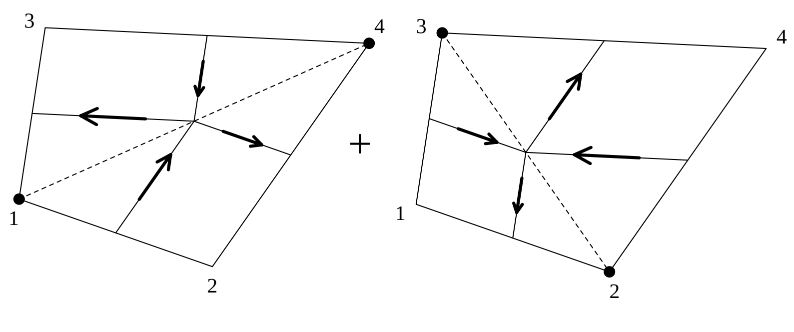
Subsequently use:

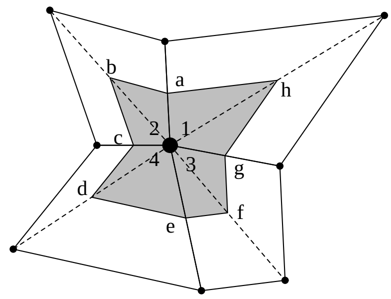
$$r_{32} = r_{34} + r_{42} \qquad r_{14} = r_{13} + r_{34} \qquad r_{41} = r_{42} + r_{21} \qquad r_{23} = r_{21} + r_{13}$$

To put the above in a more handsome form:

$$\begin{bmatrix} f_1 & f_2 & f_3 & f_4 \end{bmatrix} \begin{bmatrix} \frac{1}{2}r_{42} \times \frac{1}{2}(Q_1 + Q_2) + \frac{1}{2}r_{34} \times \frac{1}{2}(Q_1 + Q_3) \\ \frac{1}{2}r_{13} \times \frac{1}{2}(Q_1 + Q_2) + \frac{1}{2}r_{34} \times \frac{1}{2}(Q_2 + Q_4) \\ \frac{1}{2}r_{21} \times \frac{1}{2}(Q_1 + Q_3) + \frac{1}{2}r_{42} \times \frac{1}{2}(Q_3 + Q_4) \\ \frac{1}{2}r_{21} \times \frac{1}{2}(Q_2 + Q_4) + \frac{1}{2}r_{13} \times \frac{1}{2}(Q_3 + Q_4) \end{bmatrix}$$

It's a triviality, but nevertheless: a picture says more that a thousand words.





It is seen that the four pieces-of-equations correspond with four pieces of line-integrals, each of them belonging to one of the vertices. Midpoints of triangle sides are connected by lines at which the integration takes place. The heat flux at a midpoint is the average of values at the vertices.
Let's adopt another point of view now and no longer concentrate on elements but on vertices. Instead of arranging vertices around an element, elements are arranged around a vertex. Label triangle side midpoints as a, b, c, d, e, f, g, h.
It is immediately noted that the lines connecting the midsides of the triangles around a vertex, when tied together, neatly delineate a closed area, which can be interpreted as a kind of 2-D Finite Volume. Expressed in the outer product formalism, we find:

$$r_{ba} \times Q_a + r_{cb} \times Q_c + r_{dc} \times Q_c + r_{ed} \times Q_e + r_{fe} \times Q_e + r_{gf} \times Q_g + r_{hg} \times Q_g + r_{ah} \times Q_a$$

Which is the content of one equation in the Finite Element global matrix. All terms together represent a discretization of the following circular integral:

$$\sum r \times Q = \oint Q_y dx - Q_x dy$$

With help of Green's theorem, however, such a circular integral can be converted into a "volume" integral, over the area indicated in the above figure:

$$\oint Q_y dx - Q_x dy = + \iint \left[\frac{\partial Q_x}{\partial x} + \frac{\partial Q_y}{\partial y} \right] dxdy$$

Conservation of heat is integrated over a finite volume, which is wrapped around a vertex. So we have arrived at a Finite Difference method. To be more precise: at a Finite Volume method. It is remarked that this F.V. procedure has been applicable for curvilinear grids from the start.
Thus we derived a Theorem which Unifies a Finite Element and a Finite Volume method, for a rather general class of 2-D diffusion problems:
Apply a Finite Element (Galerkin) method to a mesh of quadrilaterals. Subdivide each of the quads into four (overlapping) triangles, in the two ways which

are possible. Then such a method is **equivalent** to a Finite Volume method: midsides of the triangles, around the vertex of interest, are neatly connected together, to form the boundary of a 2-D finite volume, and the conservation law is integrated over this volume.
A Unification Theorem like the above may have a couple of practical consequences, as will be investigated in the sequel.

2-D Resistor Model

Consider the two-dimensional equation (or term), which describes, for example, conduction of heat in a metal plate:

$$\frac{\partial}{\partial x}\left[-\lambda\frac{\partial T}{\partial x}\right]+\frac{\partial}{\partial y}\left[-\lambda\frac{\partial T}{\partial y}\right]=0$$

Here (x,y) = planar Cartesian coordinates, λ = conductivity, T = temperature. In general, the conductivity is also a function $\lambda(x,y)$ of the coordinates x and y . The equation is of the form:

$$\frac{\partial Q_x}{\partial x}+\frac{\partial Q_y}{\partial y}=0$$

Where:

$$Q_x=-\lambda\frac{\partial T}{\partial x} \quad ; \quad Q_y=-\lambda\frac{\partial T}{\partial y}$$

This equation has already been treated in the section "Conservation of Heat". Application of the Galerkin method there resulted in:

$$-\frac{1}{2}\left[\begin{array}{ccc} f_1 & f_2 & f_3 \end{array}\right]\left[\begin{array}{cc} y_2-y_3 & x_3-x_2 \\ y_3-y_1 & x_1-x_3 \\ y_1-y_2 & x_2-x_1 \end{array}\right]\left[\begin{array}{c} Q_x \\ Q_y \end{array}\right]$$

Discretization of Q_x and Q_y, with help of the Differentiation Matrix of a triangle, gives, in addition:

$$\left[\begin{array}{c} Q_x \\ Q_y \end{array}\right]=-\lambda\left[\begin{array}{ccc} y_2-y_3 & y_3-y_1 & y_1-y_2 \\ x_3-x_2 & x_1-x_3 & x_2-x_1 \end{array}\right]/\Delta\left[\begin{array}{c} T_1 \\ T_2 \\ T_3 \end{array}\right]$$

In order to save space, the following abbreviations will be used: $x_{ij}=x_j-x_i$, $y_{ij}=y_j-y_i$. Then the Analytical expression:

$$\frac{\partial}{\partial x}\left[-\lambda\frac{\partial T}{\partial x}\right]+\frac{\partial}{\partial y}\left[-\lambda\frac{\partial T}{\partial y}\right]$$

corresponds with the Numerical expression:

$$-\frac{1}{2}\left[\begin{array}{ccc} f_1 & f_2 & f_3 \end{array}\right]\left[\begin{array}{cc} y_{32} & x_{23} \\ y_{13} & x_{31} \\ y_{21} & x_{12} \end{array}\right] . -\lambda . \left[\begin{array}{ccc} y_{32} & y_{13} & y_{21} \\ x_{23} & x_{31} & x_{12} \end{array}\right]/\Delta\left[\begin{array}{c} T_1 \\ T_2 \\ T_3 \end{array}\right]$$

$$= + \begin{bmatrix} f_1 & f_2 & f_3 \end{bmatrix} \frac{1}{2} \begin{bmatrix} E_{11} & E_{12} & E_{13} \\ E_{21} & E_{22} & E_{23} \\ E_{31} & E_{32} & E_{33} \end{bmatrix} .\lambda/\Delta \begin{bmatrix} T_1 \\ T_2 \\ T_3 \end{bmatrix}$$

The *finite element matrix* $[E_{ij}]$ is thus defined, in our case, by:

$$\frac{1}{2} \begin{bmatrix} y_{23}.y_{23} + x_{23}.x_{23} & y_{23}.y_{31} + x_{23}.x_{31} & y_{23}.y_{12} + x_{23}.x_{12} \\ & y_{31}.y_{31} + x_{31}.x_{31} & y_{31}.y_{12} + x_{31}.x_{12} \\ \text{symmetrical} & & y_{12}.y_{12} + x_{12}.x_{12} \end{bmatrix} .\lambda/\Delta$$

A possible interpretation, for an arbitrary matrix coefficient, may be obtained as follows:

$$E_{23} = E_{32} = \frac{1}{2} \left(y_{31}.y_{12} + x_{31}.x_{12} \right) .\lambda/\Delta$$

$$= \frac{1}{2} \left[(x_2 - x_1).(x_1 - x_3) + (y_2 - y_1).(y_1 - y_3) \right] .\lambda/\Delta$$

$$= -\frac{1}{2} (\vec{r}_{12} \cdot \vec{r}_{13}).\lambda/\Delta$$

And for main diagonal elements:

$$E_{33} = \frac{1}{2} \left(y_{12}.y_{12} + x_{12}.x_{12} \right) .\lambda/\Delta$$

$$= \frac{1}{2} \left[(x_2 - x_1).(x_2 - x_1) + (y_2 - y_1).(y_2 - y_1) \right] .\lambda/\Delta$$

$$= +\frac{1}{2} (\vec{r}_{12} \cdot \vec{r}_{12}).\lambda/\Delta$$

Since any vertex of the triangle is equally important, remaining coefficients may be found by cyclic permutation of the vertex indices, according to $(1, 2, 3) \rightarrow (2, 3, 1) \rightarrow (3, 1, 2)$:

$$E_{31} = E_{13} = -\frac{1}{2} (\vec{r}_{23} \cdot \vec{r}_{21}).\lambda/\Delta$$

$$E_{12} = E_{21} = -\frac{1}{2} (\vec{r}_{31} \cdot \vec{r}_{32}).\lambda/\Delta$$

$$E_{11} = +\frac{1}{2} (\vec{r}_{23} \cdot \vec{r}_{23}).\lambda/\Delta$$

$$E_{22} = +\frac{1}{2} (\vec{r}_{31} \cdot \vec{r}_{31}).\lambda/\Delta$$

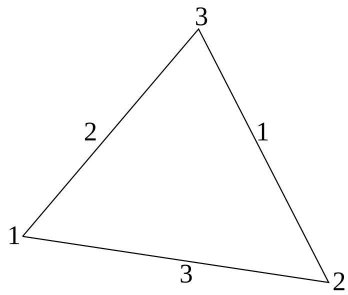
With other words: any matrix element is the *inner product* of vectors pointing from one vertex to one $(+)$ or two $(-)$ other vertices.
It is remarked that, according to one of Patankar's "Four Basic Rules" [2], namely "the rule of positive coefficients", off-diagonal terms E_{ij} with $i \neq j$ must be less than zero. This is only the case for *positive* inner products $(\vec{r}_{ki} \cdot \vec{r}_{kj})$, assuming that the determinants Δ are positive (: a convention that we have

already agreed upon). This implies that any angle of a Diffusion Triangle must be $\leq 90^o$. A special case occurs when the angle between the vectors $\vec{r}_{ki}$ and $\vec{r}_{kj} = 90$ degrees, which means that $E_{ij} = 0$. This is actually the finite difference case, on a rectangular grid: "no" triangles, but five point stars "instead".

Almost any Finite Element book starts with the assembly of resistor-like finite elements, without approximations (if one considers Ohm's law as being "exact"). Contained in [1] is a chapter about "Electrical Networks". The matrix of an electrical resistor is derived there *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.
Further define the connectivity (no coordinates!) of the resistor-network, and apply two voltages. The standard FE assembly procedure can be carried out then. Let us devise for example a triangle, built up from electrical resistors:



Opposite sides and vertices are numbered alike, which is nothing but a handsome practice. The accompanying resistor matrices are subsequently added together, to form the (finite element) resistor matrix of the triangle as a whole:

$$\begin{bmatrix} 0 & 0 & 0 \\ 0 & +1/R_1 & -1/R_1 \\ 0 & -1/R_1 & +1/R_1 \end{bmatrix} + \begin{bmatrix} +1/R_2 & 0 & -1/R_2 \\ 0 & 0 & 0 \\ -1/R_2 & 0 & +1/R_2 \end{bmatrix} + \begin{bmatrix} +1/R_3 & -1/R_3 & 0 \\ -1/R_3 & +1/R_3 & 0 \\ 0 & 0 & 0 \end{bmatrix}$$

$$= \begin{bmatrix} +1/R_2 + 1/R_3 & -1/R_3 & -1/R_2 \\ -1/R_3 & +1/R_3 + 1/R_1 & -1/R_1 \\ -1/R_2 & -1/R_1 & +1/R_1 + 1/R_2 \end{bmatrix}$$

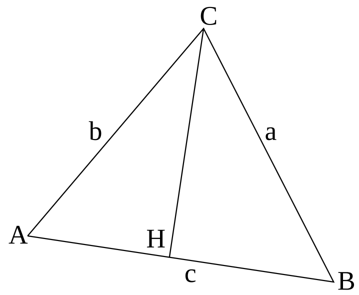
It is trivially seen that:

$$E_{11} + E_{12} + E_{13} = 0 \quad ; \quad E_{12} + E_{22} + E_{23} = 0 \quad ; \quad E_{31} + E_{32} + E_{33} = 0$$

Compare this result with our previous findings:

$$\frac{1}{2} \begin{bmatrix} y_{32}.y_{32} + x_{32}.x_{32} & y_{32}.y_{13} + x_{32}.x_{13} & y_{32}.y_{21} + x_{32}.x_{21} \\ & y_{13}.y_{13} + x_{13}.x_{13} & y_{13}.y_{21} + x_{13}.x_{21} \\ \text{symmetrical} & & y_{21}.y_{21} + x_{21}.x_{21} \end{bmatrix} .\lambda/\Delta$$

It is questioned if all terms in a matrix row sum up to zero here too. There are a myriad ways to see that this is indeed the case. According to one of Patankar's "Basic Rules", the coefficients sum up to zero without question. One can work out each term algebraically and check out. A more elegant way is via geometrical interpretation. Draw the perpendicular $\overline{CH}$ from vertex C onto $\overline{AB}$:



Take the third matrix row as an example:

$$E_{31} = E_{13} = -\frac{1}{2}c.a.cos(B).\lambda/\Delta \quad ; \quad E_{32} = E_{23} = -\frac{1}{2}c.b.cos(A).\lambda/\Delta$$

$$E_{31} + E_{32} = -\frac{1}{2}c.(\overline{AH} + \overline{BH}).\lambda/\Delta = -\frac{1}{2}c.c.\lambda/\Delta = -\,E_{33}$$

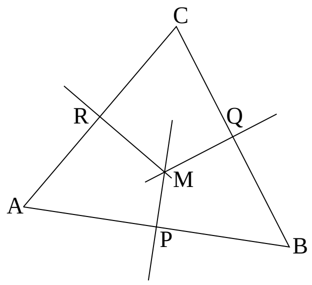
Now identify:

$$\frac{1}{2}(y_{23}.y_{31} + x_{23}.x_{31})/\Delta = -1/R_3 \quad \text{or} \quad R_3 = \frac{2\Delta/\lambda}{a.b.cos(C)}$$
$$\frac{1}{2}(y_{23}.y_{12} + x_{23}.x_{12})/\Delta = -1/R_2 \quad \text{or} \quad R_2 = \frac{2\Delta/\lambda}{a.c.cos(B)}$$
$$\frac{1}{2}(y_{31}.y_{12} + x_{31}.x_{12})/\Delta = -1/R_1 \quad \text{or} \quad R_1 = \frac{2\Delta/\lambda}{b.c.cos(A)}$$

Thus we can consider the 3×3 matrix for diffusion at a triangle as a superposition of one-dimensional resistor-like elements (an outstanding example of substructuring, anyway). When assembling these triangle matrices into the global system, most resistors have to be replaced by two parallel resistors, one resistor for each side of a triangle, according to the law: $1/R = 1/R_a + 1/R_b$. Exceptions are at the boundary. The main diagonal term in a matrix equals the sum of the off-diagonal terms. This result can be used as follows: account *only* for the off-diagonal terms in the first place. At the very end of the F.E. assembly procedure, sum up each matrix row, in order to obtain the main diagonal elements.

Voronoi Regions

Let A, B, C be the vertices of a triangle, as depicted in the Figure below.
Let P be the middle of AB. Draw the median through P perpendicular to $\overline{AB}$.
Let Q be the middle of BC. Draw the median through Q perpendicular to $\overline{BC}$.
Let R be the middle of AC. Draw the median through R perpendicular to $\overline{AC}$.
Let the coordinates of A be given by (x_A, y_A).
Let the coordinates of B be given by (x_B, y_B).
Let the coordinates of C be given by (x_C, y_C).



It is well known from planar geometry that the perpendicular medians through P, Q and R have a common intersection point M. The equations of these lines are given by:

$$\begin{array}{rl} \overline{PM}: & (x,y) = \frac{1}{2}(x_A + x_B, y_A + y_B) + \gamma.(y_B - y_A, x_A - x_B) \\ \overline{QM}: & (x,y) = \frac{1}{2}(x_B + x_C, y_B + y_C) + \alpha.(y_C - y_B, x_B - x_C) \\ \overline{RM}: & (x,y) = \frac{1}{2}(x_C + x_A, y_C + y_A) + \beta.(y_A - y_C, x_C - x_A) \end{array}$$

The intersection point M is associated with values for γ , α and β, which are labelled as γ_M , α_M and β_M . At first γ_M and α_M will be calculated, by:

$$\frac{1}{2}(x_A + x_B, y_A + y_B) + \gamma_M.(y_B - y_A, x_A - x_B) =$$
$$\frac{1}{2}(x_B + x_C, y_B + y_C) + \alpha_M.(y_C - y_B, x_B - x_C)$$

Giving two equations with two unknowns:

$$\begin{array}{l} \frac{1}{2}(x_A + x_B) + \gamma_M.(y_B - y_A) = \frac{1}{2}(x_B + x_C) + \alpha_M.(y_C - y_B) \\ \frac{1}{2}(y_A + y_B) + \gamma_M.(x_A - x_B) = \frac{1}{2}(y_B + y_C) + \alpha_M.(x_B - x_C) \end{array} \quad \Longleftrightarrow$$

$$\begin{bmatrix} y_B - y_A & -(y_C - y_B) \\ -(x_B - x_A) & x_C - x_B \end{bmatrix} \begin{bmatrix} \gamma_M \\ \alpha_M \end{bmatrix} = \frac{1}{2} \begin{bmatrix} x_C - x_A \\ y_C - y_A \end{bmatrix}$$

The matrix at the left side can be inverted, resulting in:

$$\begin{bmatrix} \gamma_M \\ \alpha_M \end{bmatrix} = \begin{bmatrix} x_C - x_B & y_C - y_B \\ x_B - x_A & y_B - y_A \end{bmatrix} . \frac{1}{2} \begin{bmatrix} x_C - x_A \\ y_C - y_A \end{bmatrix} / \Delta$$

Where:

$$\Delta = (x_C - x_B)(y_B - y_A) - (x_B - x_A)(y_C - y_B)$$

Hence:

$$\gamma_M = \frac{1}{2}\left[(x_C - x_B)(x_C - x_A) + (y_C - y_B)(y_C - y_A)\right]/\Delta$$

Define $\vec{r}_{KL} = (x_L - x_K, y_L - y_K)$. Then, with an analogous calculation for α_M and an educated guess for β_M, we find:

$$\gamma_M = \frac{1}{2}(\vec{r}_{CA} \cdot \vec{r}_{CB})/\Delta$$
$$\alpha_M = \frac{1}{2}(\vec{r}_{AB} \cdot \vec{r}_{AC})/\Delta$$
$$\beta_M = \frac{1}{2}(\vec{r}_{BA} \cdot \vec{r}_{BC})/\Delta$$

Compare this with our findings in '2-D Resistor Model':

$$E_{12} = E_{21} = -\frac{1}{2}(\vec{r}_{31} \cdot \vec{r}_{32}).\lambda/\Delta = -1/R_3$$
$$E_{23} = E_{32} = -\frac{1}{2}(\vec{r}_{12} \cdot \vec{r}_{13}).\lambda/\Delta = -1/R_1$$
$$E_{31} = E_{13} = -\frac{1}{2}(\vec{r}_{23} \cdot \vec{r}_{21}).\lambda/\Delta = -1/R_2$$

With $1 \sim A$, $2 \sim A$, $3 \sim C$, it is concluded that:

$$\lambda.\gamma_M = 1/R_3 \quad ; \quad \lambda.\alpha_M = 1/R_1 \quad ; \quad \lambda.\beta_M = 1/R_2$$

Assuming that our triangles have non-obtuse angles, we can read from the figure that $\gamma_M, \alpha_M, \beta_M > 0$. In this case:

$$|\lambda.\gamma_M.(y_B - y_A, x_A - x_B)| = 1/R_3.\overline{AB} = \lambda.\overline{PM} \quad \Longrightarrow$$

$$R_3 = \frac{\overline{AB}}{\lambda.\overline{PM}} = \frac{\text{"length" of } R_3}{\text{conductivity} \times \text{"diameter" of } R_3}$$

In very much the same way we can prove that:

$$R_1 = \frac{\overline{BC}}{\lambda.\overline{QM}} = \frac{l_1}{\lambda.O_1} \quad ; \quad R_2 = \frac{\overline{CA}}{\lambda.\overline{RM}} = \frac{l_2}{\lambda.O_2}$$

Where: $l =$ length, $O =$ diameter. This gives us a lucid physical interpretation of the resistances R_k, as they are associated with the linear triangle. It is also seen now why obtuse angles are more or less unacceptable. In this case one of the resistances will become *negative*, meaning that a (heat) current will flow from a place with low temperature to a place with high temperature, thus violating the Second Law of Thermodynamics. By "more or less" we mean that

any such obtuse angle should be compensated by a sufficiently sharp one in the opposite triangle, in such a way that the sum $1/R_a + 1/R_b$ of their respective contributions shall be positive.
Having said all this, we would like to generalize the above result, in order to include Diffusion *as well as* Convection. An obvious way to do this, is to make use of the Resistor model, since the latter effectively sets up a link to the much simpler *one-dimensional* theory. As follows. When considering *any* flux through $\overline{PM}$, the same line segment is associated with a normal vector $\vec{PM}$ which is perpendicular to it. Its length is given by:

$$\overline{PM} = \gamma_M |(y_B - y_A, x_A - x_B)| = \gamma_M |(x_B - x_A, y_B - y_A)| = \gamma_M \overline{AB}$$

This is nice, because $\vec{PM}$ has also the same direction as $\vec{AB}$. Thus we can put:

$$\vec{PM} = \gamma_M \vec{AB} = \frac{1}{2}(\vec{r}_{31} \cdot \vec{r}_{32})/\Delta \, . \, \vec{r}_{12}$$

In very much the same way we find:

$$\vec{QM} = \frac{1}{2}(\vec{r}_{12} \cdot \vec{r}_{13})/\Delta \, . \, \vec{r}_{23}$$
$$\vec{RM} = \frac{1}{2}(\vec{r}_{23} \cdot \vec{r}_{21})/\Delta \, . \, \vec{r}_{31}$$

The Diffusive flux from (1) to (2) through resistor $\overline{AB}$ is:

$$I_{12}^D = (T_1 - T_2)/R_3 = \frac{\lambda \overline{PM}}{\overline{AB}}(T_1 - T_2) = \frac{1}{2}(\vec{r}_{31} \cdot \vec{r}_{32})/\Delta . \lambda (T_1 - T_2)$$

Here $(T_1 - T_2)$ is the temperature-difference between A and B, λ = thermal conductivity $(J/m/s/K)$. Analogously, the *Convective* flux through resistor $\overline{AB}$ is the heat flow coming from (1). It streams through the area $\overline{PM}$ and mixes with the fluid in (2). The net effect is:

$$I_{12}^C = \rho . c . (\vec{v} \cdot \vec{PM}) . (T_1 - T_2)$$

Here ρ = density (kg/m^3), c = heat capacity $(J/kg/K)$, $\vec{v}$ = velocity (m/s), T_k = local temperature of the fluid (K). Continuing:

$$I_{12}^C = \rho . c . \frac{1}{2}(\vec{r}_{31} \cdot \vec{r}_{32})/\Delta . (\vec{v} \cdot \vec{r}_{12})(T_1 - T_2)$$

So the expressions for Diffusive flux and Convective flux are very much alike:

$$I_{12}^D = \lambda . G_{12} . (T_1 - T_2)$$
$$I_{12}^C = \rho . c . (\vec{v} \cdot \vec{r}_{12}) . G_{12} . (T_1 - T_2)$$

Where $G_{12} = \frac{1}{2}(\vec{r}_{31} \cdot \vec{r}_{32})/\Delta$ is a purely geometrical factor, which embodies the geometry of the triangle. The quotient of Convective and Diffusive flux is entirely independent of that two-dimensional geometry:

$$P = \rho.c.(\vec{v} \cdot \vec{r}_{ij})/\lambda$$

Here $\vec{r}_{ij} = \vec{r}_j - \vec{r}_i$ = vector from (i) to (j). The projection of the velocity vector on a direction vector replaces the quantity $\rho.c.v.dx/\lambda$ in the one-dimensional theory. Therefore, P may be interpreted, again, as a dimensionless *local Péclet number*.

Now the time has come to generalize a result from Patankar's book [2], namely the formulas (5.47) from 5.2-7 *A Generalized Formulation*:

$$\begin{aligned} a_E &= D_e A(|P_e|) + max(-F_e, 0) \\ a_W &= D_w A(|P_w|) + max(+F_w, 0) \\ a_P &= a_E + a_W + (F_e - F_w) \end{aligned}$$

It will be assumed in the sequel that the continuity equation is valid, hence $F_e - F_w = 0$. The formulas (5.47) are accompanied with several expressions for the function $A(|P|)$, as given in [2] by *Table 5.2 The function $A(|P|)$ for different schemes*:

Central difference	$A(\|P\|) = 1 - 0.5\|P\|$
Upwind	$A(\|P\|) = 1$
Hybrid	$A(\|P\|) = max(0, 1 - 0.5\|P\|)$
Power law	$A(\|P\|) = max(0, (1 - 0.1\|P\|)^5)$
Exponential (exact)	$A(\|P\|) = \|P\| / [exp(\|P\|) - 1]$

Switching to the Finite Element viewpoint means insisting that assembly of the F.D. equations shall be done with F.E. matrices, instead of row by row. Here comes our educated guess of such a matrix:

$$\begin{bmatrix} E_{11} & E_{12} \\ E_{21} & E_{22} \end{bmatrix} = \begin{bmatrix} +a_E & -a_E \\ -a_W & +a_W \end{bmatrix}$$

Since we must be certain that this is indeed the correct matrix, assemble two of these to a complete equation - which is at the row in the middle - and associate the proper unknowns:

$$\begin{bmatrix} +a_E & -a_E & 0 \\ -a_W & +a_W + a_E & -a_E \\ 0 & -a_W & +a_W \end{bmatrix} \begin{bmatrix} \phi_W \\ \phi_P \\ \phi_E \end{bmatrix}$$

Meanwhile, we have found Linear Triangle equivalents for each of the terms that constitute a_E and a_W:

$$\begin{aligned} D_{e/w} &= G_{ij}\ \lambda \\ P_{e/w} &= \rho.c.(\vec{v} \cdot \vec{r}_{ij})/\lambda \\ F_{e/w} &= G_{ij}\ \rho.c.(\vec{v} \cdot \vec{r}_{ij}) \end{aligned}$$

Physical quantities are evaluated at (e/w), corresponding with the middle of the accompanying resistor elements. A significant detail is the difference between the $\pm$ signs in:

$$-E_{12} = a_E = D_e A(|P_e|) + max(-F_e, 0)$$
$$-E_{21} = a_W = D_w A(|P_w|) + max(+F_w, 0)$$

No reason to bother, however, because when evaluated at the same place:

$$+F_w = \rho.c.(\vec{v} \cdot \vec{r}_{12}) = -\rho.c.(\vec{v} \cdot \vec{r}_{21}) \quad \Longrightarrow \quad -E_{ij} = D_{ij} A(|P_{ij}|) + max(-F_{ij}, 0)$$

Further simplification will be achieved by assuming that λ is a constant and dividing the quantities $D_{e/w} = D_{ij}$ and $F_{e/w} = F_{ij}$ by this conductivity:

$$D_{ij}/\lambda = G_{ij}$$
$$P_{ij} = \rho.c.(\vec{v} \cdot \vec{r}_{ij})/\lambda$$
$$F_{ij}/\lambda = G_{ij} \; P_{ij}$$

The end result is an F.E. matrix which is suitable for Convection And Diffusion:

$$\begin{bmatrix} +E_{12} & -E_{12} \\ -E_{21} & +E_{21} \end{bmatrix} \qquad \text{where:} \qquad E_{ij} = G_{ij} \; [A(|P_{ij}|) \; + \; max(0, -P_{ij})]$$

It is remarked that the above generalization is *faithful*, meaning that it is reduced *exactly* to Patankar's original scheme, when specialized for a rectangular grid. (Such a thing is not accomplished, strangely enough, with the F.E. formulation as devised by Patankar himself in [2] paragraph 8.4-3).
Our theory is accompanied with a sample program, which has been coded in Delphi Pascal. Heat Transfer is described there by the following PDE:

$$Pe \left[u\frac{\partial T}{\partial x} + v\frac{\partial T}{\partial y} \right] - \left[\frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2} \right] = 0$$

Pe = overall Péclet number, (x, y) = normed coordinates, (u, v) = normed velocity field, T = temperature.
My favorite sample flow field is given by the conformal (complex) mapping $\zeta = z^2/2$. Taking the real and the complex part of it gives rise to a potential function ϕ and a stream function ψ respectively:

$$\phi(x, y) = \frac{1}{2}(x^2 - y^2) \quad \text{and} \quad \psi(x, y) = x.y$$

Contours of the functions ϕ and ψ form two systems of orthogonal hyperbolas. These hyperbolas are mutually orthogonal where they intersect. The points of intersection form the basis of a triangular mesh. They are found as follows:

$$\frac{1}{2}(x^2 - y^2) = A \quad \text{and} \quad x.y = B \quad \Longrightarrow \quad \frac{1}{2}x^2 - \frac{1}{2}(B/x)^2 = A$$

$$\Longrightarrow \quad x^4 - 2Ax^2 - B^2 = 0 \quad \Longrightarrow \quad x^2 = \sqrt{A^2 + B^2} \pm |A|$$

$$\Longrightarrow \quad x = \sqrt{\sqrt{A^2 + B^2} \pm |A|} \quad \text{and} \quad y = \sqrt{x^2 - 2A}$$

The domain of interest is bounded by x-axis, y-axis and relevant outer pieces of the hyperbolas. The velocity field is derived from either the potential or the stream function:

$$u = \frac{\partial \phi}{\partial x} = \frac{\partial \psi}{\partial y} = x \quad \text{and} \quad v = \frac{\partial \phi}{\partial y} = -\frac{\partial \psi}{\partial x} = -y$$

Our theory seems to be finished herewith. The rest is a matter of technology. Accompanying software is supposed to be found at:

`http://hdebruijn.soo.dto.tudelft.nl/jaar2004/purified.zip`

However, the precise location of the ZIP file may be subject to change without prior notification. Remember: anything **free** comes without guarantee !

References

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

[2] S.V. Patankar, "Numerical Heat Transfer and Fluid Flow", Hemisphere PublishingCompany U.S.A. 1980.