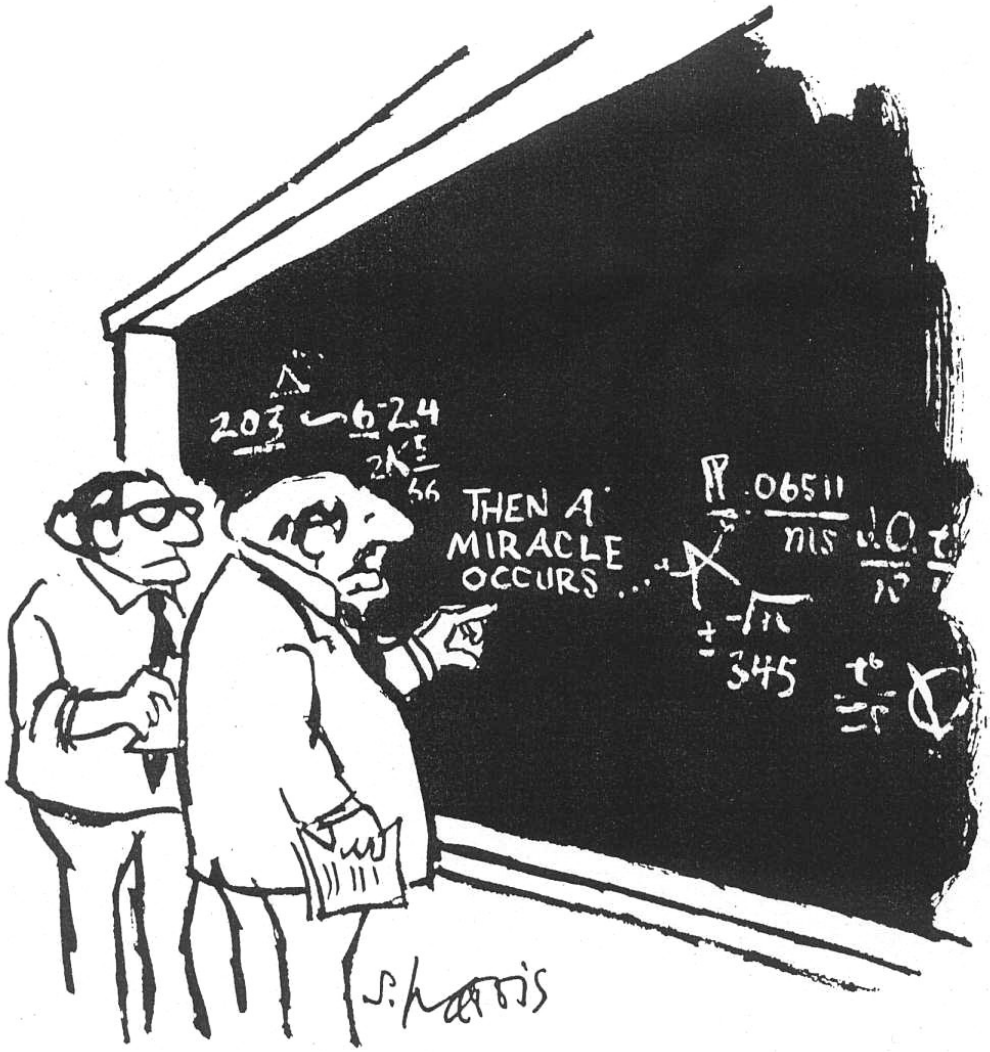
INSIDE FINITE ELEMENTS FOR OUTSIDERS

Groundwater flow, stationary and transient conditions, contaminant transport, heat transport, stress strain.

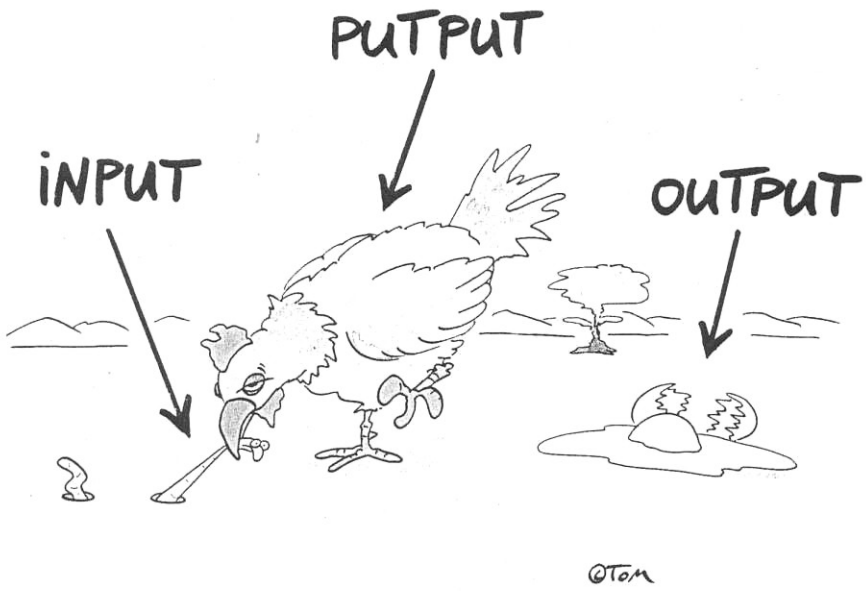


"I THINK YOU SHOULD BE MORE EXPLICIT HERE IN STEP TWO."

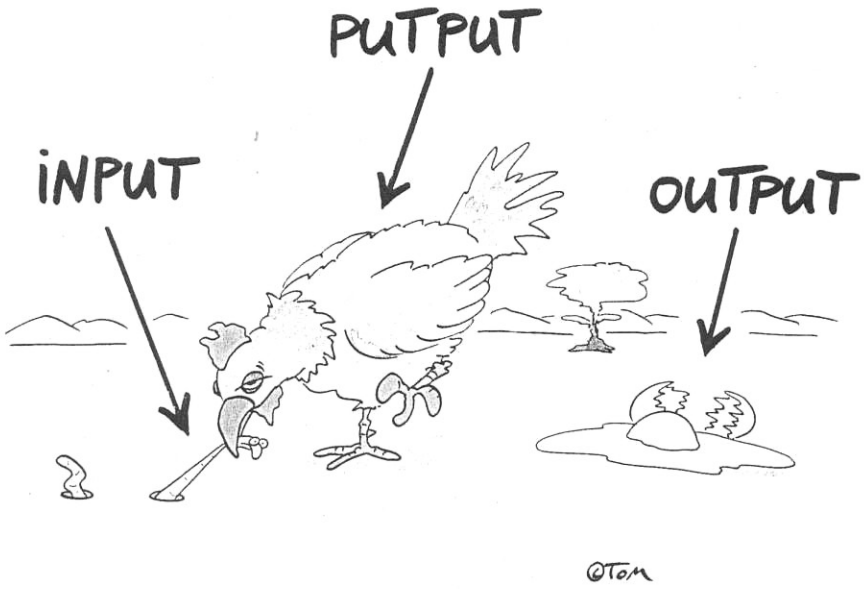
Harris´ berühmtester Cartoon. „Ich denke, Sie sollten den zweiten Schritt besser erklären"

UNDERSTANDING STEP 2

Index



STEP 2: UNDERSTANDING THE PUTPUT



Chris McDermott.
Center for Applied Geology (ZAG)
Tübingen 7.10.2003
Chris.mcdermott@uni-tuebingen.de

Special thanks to PD. Rudolf Liedl who spent a lot of time helping me to get to grips with the mathematical formulations.

Inside Finite Elements for Outsiders

Application to Groundwater Flow, Contaminant transport in Groundwater, Heat transport in groundwater, Stress and Strain applications.

1. Introduction

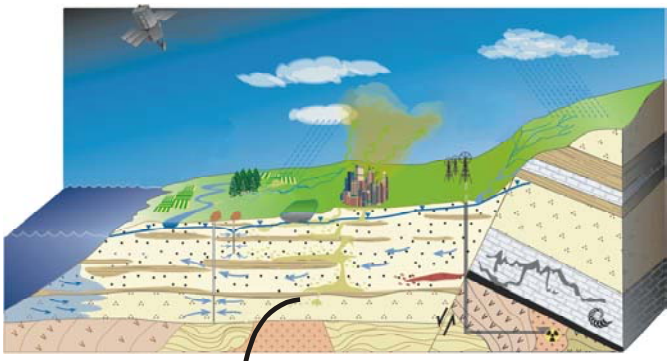
This paper is designed for those who do not come from an Engineering or Mathematical back ground and need to get to grips with Finite Element computing. For those of you who are not sure what a Gauss Quadrature is, a Gauss Greens or Gauss-Ostrogradskian integral theorem is and thought to date that Galerkin was actually a special name for a type of Cucumber or Gerkin then this is the right thing for you. It is written by someone who had to spend a lot of time wading through mathematical expressions written in Greek and translated them into common sense, and who got quite annoyed at expressions like "it is easy to show that" or "obviously..". Its for those of you who felt you were skating on very thin ice. The ice will get a bit thicker hopefully, but you could still fall through it:- at least you should have an idea why you fell through it.

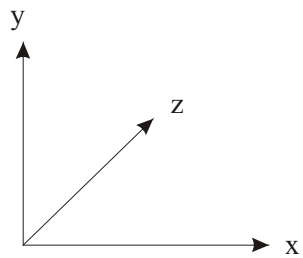
Two reference publications in particular are recommended for their practical approach and use of understandable examples: "Groundwater Modelling by the Finite Element Method" by Jonathan Istok (thankyou!!) and lecture notes prepared by Felipa, Carlos A, University of California, available under http://titan.colorado.edu/courses.d/IFEM.d/ . After coming to grips with the information presented here and in detail in these publications you can tackle more standard text books such as that by Zienkiewicz and begin to appreciate the compact and clear presentation presented there of various finite element solutions.

Examples worked out in excel for one dimensional modelling of saturated and transient groundwater flow, contaminant and heat transport, two dimensional stress strain and saturated groundwater flow are given in and available in an accompanying excel file to help you follow what is going on. You can play around with the excel file, I have got the original so you can't "break it."

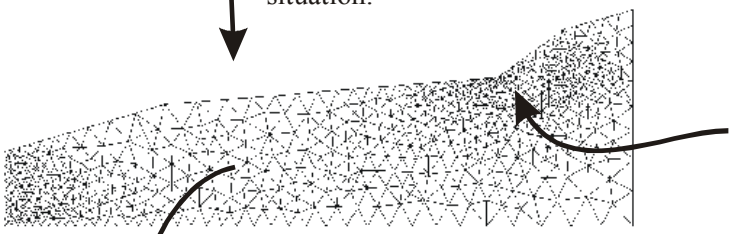
2. Object to be modelled to finite element mesh.

The object / area (from now on area) to be modelled is divided into smaller elements linked in a mesh.. finite elements. The shape of the element is variable, bars, triangle, squares, tetrahedral and cubes are most commonly used. The boundaries of the element are defined by nodes usually at the corners of the elements, but sometimes also along the boundary of the elements and within the element. For our purposes the "inner node" elements will not be discussed here. The nodes are numbered and assigned natural coordinates of the area in question. The elements are numbered and the nodes assigned to each element recorded. More elements are generated in places of special interest, or where there are expected to be higher than normal changes in the parameters being included in the model. This process, known as discretization or meshing is illustrated in Figure 2-1.



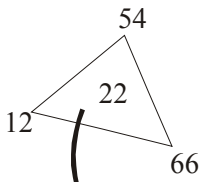


Approximation of real life situation.



In areas of interest, or points where large differences in parameters are expected the mesh is made finer.

Mesh made up of several finite elements described by the nodes and the coordinates of the nodes in the natural coordinate system.



Element 22
Nodes

Number	x coord.	y coord.	z coord
54	100	110	0
12	90	100	0
66	110	95	0

Figure 2-1: Dicretization / meshing of area to be modelled.

Once the area has been discretized the construction of a mathematical model to describe the processes being investigated is undertaken. This mathematical model is unique to the process being simulated, similar processes having similar expressions. An example is looking for the head (measure of water pressure) distribution in a area, where only boundary values of the head are known. Illustrated in Figure 2-2, or a rock under applied stress, Figure 2-3.

What is interesting about these scenarios is that the same net is used in both. These conditions will be used to provide a 2D example of groundwater flow, and of stress strain analysis to get you used to what is going on.

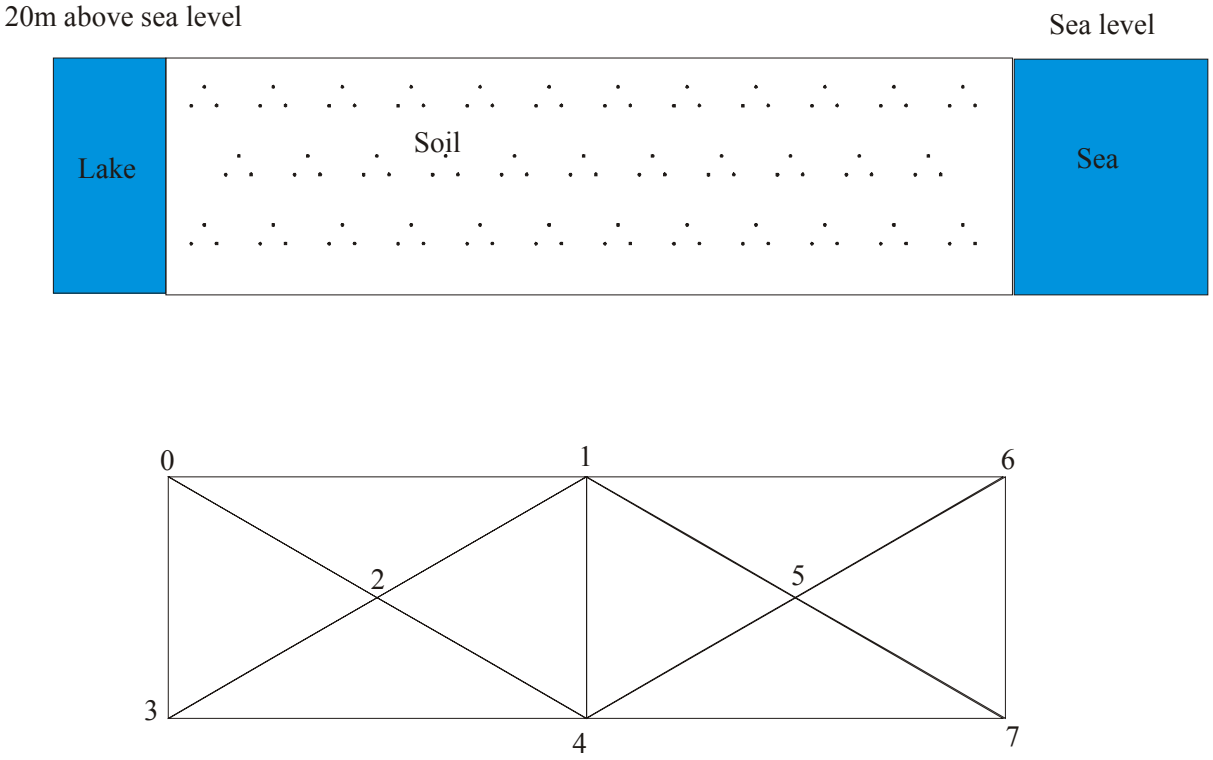


Figure 2-2: Boundary conditions and discetization of a simple model for groundwater flow.

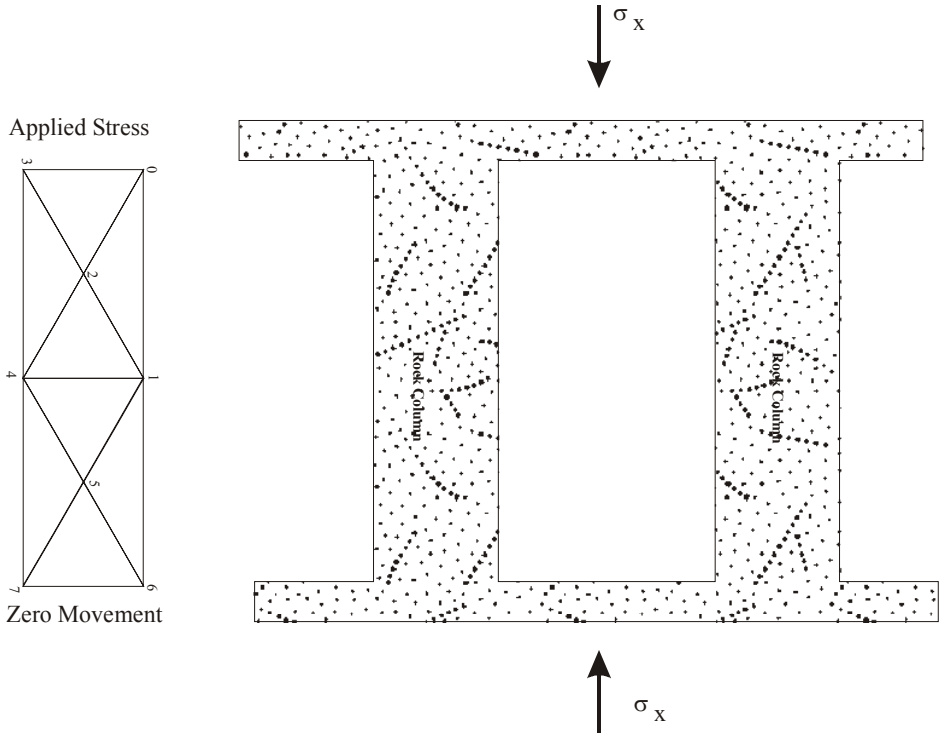


Figure 2-3: Boundary conditions and discretization for a simple rock column model

3. Don't Panic: Principle behind Finite Element Calculations

The principle behind the application of the FE (Finite Element) technique is that everything is broken down into matrices representing the governing equations, which are then solved for the unknown values. The principle equation given is

Eq. (3.1) $\mathbf{Ku} = \mathbf{f}$

Where **u** contains some variable related to **f** through the matrix **K**. In groundwater **K** would be the Conductance Matrix, **u** would be the heads and **f** would be the flux. In stress and strain analysis **K** is the stiffness matrix, **u** are the displacements and **f** are the forces. How we get the values for K is discussed later, but in principle we can see from above that

Eq. (3.2) $\mathbf{u} = \mathbf{K}^{-1}\mathbf{f}$

so if **f** is known we can solve for **u**, or if **u** is known we can solve for **f**. The difficulties start in understanding how **K**, **u** and **f** are constructed. That will be most of the rest of this paper. For this stage let us take a look at Figure 3-1. What do we know?. Let u be the displacement, and f be the forces involved. The finite element mesh approximation is shown in Figure 3-2. We see we have 8 nodes, 0 to 7 (starting at 0 because C++ vectors and matrices with the first reference being 0), and in this case 7 elements.

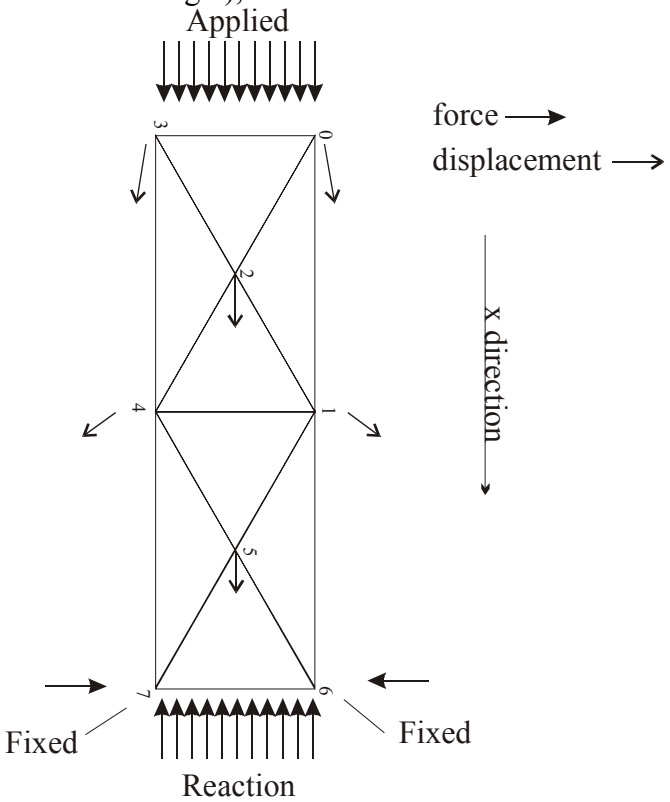


Figure 3-1: Stress applied to the top of the rock column causes deformation.

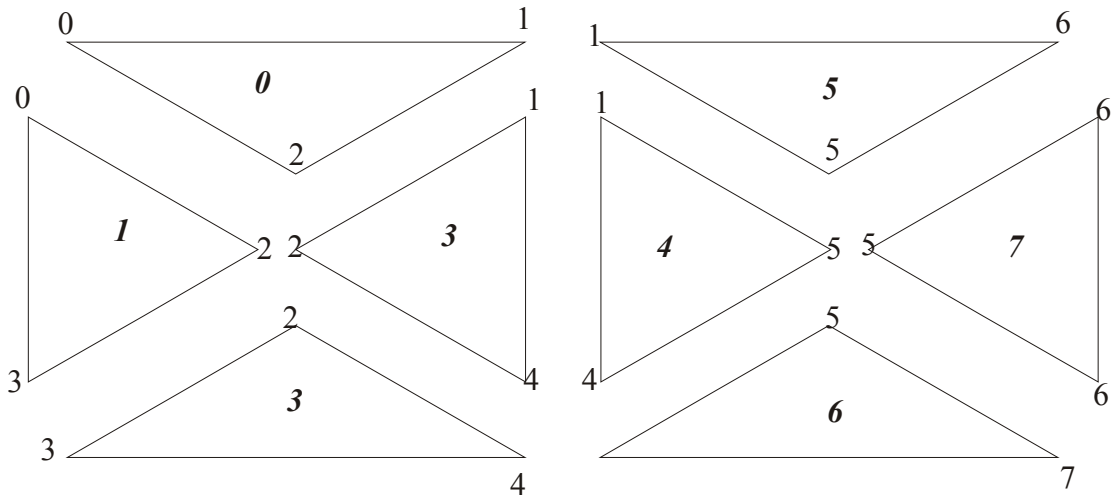


Figure 3-2: Mesh in detail.

Let us know assign a simple coordinate system, where the units of x and y are metres and the node 3 is at the position 0,0. We can then define all the nodes of this mesh and the elements as illustrated in table 1.

Table 1: Nodal Coordinates

Node	x	y	Element	Nodes
0	0	2	0	0 2 1
1	2	2	1	3 2 0
2	1	1	2	3 4 2
3	0	0	3	2 4 1
4	2	0	4	4 5 1
5	3	1	5	1 5 6
6	4	2	6	4 7 5
7	4	0	7	5 7 6

Dealing with forces we need to consider both the x direction and the y direction. Likewise we have movement in both the x and y direction. Therefore every node has an x component and a y component. In a three dimensional system this would also include a z coordinate. Many systems can be approximated in 2D, by assuming a unit thickness of z the necessity to include variations in the z direction is removed.

The force vector **f** and the movement vector **u** are then composed of an x and a y component for every node:-

$$\mathbf{u} = \begin{bmatrix} u_{0x} \\ u_{0y} \\ u_{1x} \\ u_{1y} \\ u_{2x} \\ u_{2y} \\ u_{3x} \\ u_{3y} \\ u_{4x} \\ u_{4y} \\ u_{5x} \\ u_{5y} \\ u_{6x} \\ u_{6y} \\ u_{7x} \\ u_{7y} \end{bmatrix} \qquad \mathbf{f} = \begin{bmatrix} f_{0x} \\ f_{0y} \\ f_{1x} \\ f_{1y} \\ f_{2x} \\ f_{2y} \\ f_{3x} \\ f_{3y} \\ f_{4x} \\ f_{4y} \\ f_{5x} \\ f_{5y} \\ f_{6x} \\ f_{6y} \\ f_{7x} \\ f_{7y} \end{bmatrix} \qquad \text{Eq. (3.3)}$$

Looking at the sketch, Figure 3-1, we can see that from the forces we are applying and the movement possibilities we can define Eq. (3.3). Whether this is physical reality is questionable, but will do as our example (In reality the rock below the column would also deform). If I know **K**, I can then solve the whole system for the unknown values of **f** and **u**. From this solution I can then define a number of other values, such as strain and stress in the actual elements. Should this have been a groundwater example, the unknowns would have either been heads or flux, I would get a solution for all heads and flux, and from the heads I could derive the gradient dh/dx, which coupled with the permeability then gives me ground water velocity. You don't need to understand this at this stage, but just see the usefulness.

$$\mathbf{u} = \begin{bmatrix} u_{0x} \\ u_{0y} \\ u_{1x} \\ u_{1y} \\ u_{2x} \\ u_{2y} \\ u_{3x} \\ u_{3y} \\ u_{4x} \\ u_{4y} \\ u_{5x} \\ u_{5y} \\ u_{6x} = 0 \\ u_{6y} = 0 \\ u_{7x} = 0 \\ u_{7y} = 0 \end{bmatrix} \qquad \mathbf{f} = \begin{bmatrix} f_{0x} = \sigma_x \\ f_{0y} = 0 \\ f_{1x} = 0 \\ f_{1y} = 0 \\ f_{2x} = 0 \\ f_{2y} = 0 \\ f_{3x} = \sigma_x \\ f_{3y} = 0 \\ f_{4x} = 0 \\ f_{4y} = 0 \\ f_{5x} = 0 \\ f_{5y} = 0 \\ f_{6x} \\ f_{6y} \\ f_{7x} \\ f_{7y} \end{bmatrix} \qquad \text{Eq. (3.4)}$$

Boundary conditions and initial conditions included.

4. Development of the Finite Element Formulation.

There is a different mathematical solution for each process to be modelled, although in principle the steps are the same. Basically an expression is found which defines the parameters we are interested in at every node. Below are the expressions for:-

Saturated Steady State Groundwater Flow Eq. (4.1)

$$\frac{\partial}{\partial x}\left(K_x\frac{\partial h}{\partial x}\right)+\frac{\partial}{\partial y}\left(K_y\frac{\partial h}{\partial y}\right)+\frac{\partial}{\partial z}\left(K_z\frac{\partial h}{\partial z}\right)=0 \qquad \text{Eq. (4.1)}$$

K_x is the permeability in the x direction.

Saturated Transient Groundwater Flow Eq. (4.2)

$$\frac{\partial}{\partial x}\left(K_x\frac{\partial h}{\partial x}\right)+\frac{\partial}{\partial y}\left(K_y\frac{\partial h}{\partial y}\right)+\frac{\partial}{\partial z}\left(K_z\frac{\partial h}{\partial z}\right)=\frac{\partial h}{\partial t}S_s \qquad \text{Eq. (4.2)}$$

S_s is the storage coefficient.

Unsaturated Steady State Groundwater Flow Eq. (4.3)

$$\frac{\partial}{\partial x}\left(K_x(\psi)\frac{\partial \psi}{\partial x}\right)+\frac{\partial}{\partial y}\left(K_y(\psi)\frac{\partial \psi}{\partial y}\right)+\frac{\partial}{\partial z}\left(K_z(\psi)\left(\frac{\partial \psi}{\partial z}+1\right)\right)=0 \qquad \text{Eq. (4.3)}$$

ψ is the degree of saturation.

Unsaturated Transient Groundwater Flow Eq. (4.4)

$$\frac{\partial}{\partial x}\left(K_x(\psi)\frac{\partial \psi}{\partial x}\right)+\frac{\partial}{\partial y}\left(K_y(\psi)\frac{\partial \psi}{\partial y}\right)+\frac{\partial}{\partial z}\left(K_z(\psi)\left(\frac{\partial \psi}{\partial z}+1\right)\right)=C(\psi)\frac{\partial \psi}{\partial t} \qquad \text{Eq. (4.4)}$$

$C(\psi)$ is the moisture capacity

Solute Transport Equation Eq. (4.5)

$$\begin{aligned}\frac{\partial(\theta C)}{\partial t} &= D_x\frac{\partial^2}{\partial x^2}(\theta C)+D_y\frac{\partial^2}{\partial y^2}(\theta C)+D_z\frac{\partial^2}{\partial z^2}(\theta C)\\ &-\frac{\partial}{\partial x}(v_x C)-\frac{\partial}{\partial y}(v_y C)-\frac{\partial}{\partial z}(v_z C)-\frac{\partial}{\partial t}(\rho_b K_d C)\\ &-\lambda(\theta C+\rho_b K_d C)\end{aligned} \qquad \text{Eq. (4.5)}$$

C is the solute concentration, θ is the volumetric water content, K_d the sorbtion coefficient, λ is the solute decay coefficient, ρ_b is the bulk density, and D is the diffusion coefficient.

Heat Transport Eq. (4.6)

$$c\rho\frac{\partial T}{\partial t} = D_x\frac{\partial^2 T}{\partial x^2} + D_y\frac{\partial^2 T}{\partial y^2} + D_z\frac{\partial^2 T}{\partial z^2} - c^w\rho^w v_x\frac{\partial T}{\partial x} - c^w\rho^w v_y\frac{\partial T}{\partial y} - c^w\rho^w v_z\frac{\partial T}{\partial z} - \rho Q_T \qquad \text{Eq. (4.6)}$$

c is the heat capacity, ρ is the density, D is the heat diffusion dispersion tensor of the porous medium, T is the temperature, and Q is the source term.

Deformation Eq. (4.7)

Expressed for the elements:

$$K^e u^e = f_M^e + f_I^e \qquad \text{Eq. (4.7)}$$

where f_M^e represents mechanical forces due operating on the object, and f_I^e are classed as initial forces and include thermal strain, body forces, and existent stress fields.

Development of the equations:-
This text is designed to give an introduction into the application of the finite element technique to the solution of the equations Eq. (4.1) to Eq. (4.7) and not to prove the equations themselves. This is better left to Kolditz (2000), de Marsily (1981), or very easily readable Fetter (1993). The stress strain relationships are developed in Zienkiewick & Taylor (2002) and more easily understandable in Felipa, Carlos A lecture notes.

5. Conversion of process equations into Finite Element Formulations

We will start with the saturated groundwater flow equation, given as

$$\frac{\partial}{\partial x}\left(K_x \frac{\partial h}{\partial x}\right)+\frac{\partial}{\partial y}\left(K_y \frac{\partial h}{\partial y}\right)+\frac{\partial}{\partial z}\left(K_z \frac{\partial h}{\partial z}\right)=0 \qquad \text{Eq. (5.1)}$$

This equation states that the flow into and out of a volume in space (we cold consider it as one of the elements) is constant. In vector terms this is given the term

$$div(flux)=0 \qquad \text{Eq. (5.2)}$$

here the flux is the velocity of the water multiplied by the area through which it is flowing.

Let us consider the one dimensional case, we will derive a finite element formulation for it. Let Kx be constant in the element, although it can vary from element to element then:

$$K_x \frac{\partial^2 h}{\partial x^2}=0 \qquad \text{Eq. (5.3)}$$

The values of the heads at the boundary conditions are known, but the values of the heads throughout the area being modelled are not known. We want to come up with the a finite element formulation as follows:-

$$\mathbf{Ku = R} \qquad \text{Eq. (5.4)}$$

K will be our conductance matrix related to the permeability, u will be the heads throughout the network and R will be the fluxes in and out of the nodes. Now if we consider this carefully R should be 0, as the fluxes coming in will match the fluxes going out for steady state flow, so we see we need a solution for u where all the fluxes equal 0.

To get solution for **u**, which is the distribution of heads across the network, we need to be able to interpolate the head values between nodes. This is the first introduction to the "interpolation function", or "shape function" used for predicting the unknown value of h along the element. In the correct solution of Eq. (5.4) the value of R is 0 for all points except where there is flow into or out of the area being modelled. Using the interpolated function there may be a small residual error.

Let us take the 1D model in Figure 5-1: 1D Model

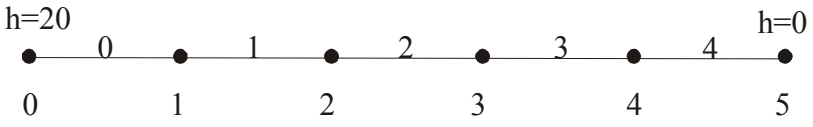


Figure 5-1: 1D Model

The heads on the left and on the right are known, those of nodes 1,2,3,4 are not known.

The interpolation functions are really a weighting applied to each of the nodal values of an element according to position of the point being examined in the element. In our example the interpolated value of h is given by

$$\hat{h} = \sum_i^m N_i h_i \qquad \text{Eq. (5.5)}$$

For a two noded element there are then two terms to this equation, for a three noded element (triangle) there are three terms, and so on. For the one dimensional example we have two nodes: therefore two terms.

$$\hat{h} = \frac{x_2 - x}{x_2 - x_1} h_1 + \frac{x - x_1}{x_2 - x_1} h_2 \qquad \text{Eq. (5.6)}$$

Here node 1 has a lower x value than node 2, and we are moving from lower x to higher x values. All the values of x are given in the real coordinate system, the values of h refer to the nodal values of h, x1 is the coordinate of node 1, x2 the coordinate of x2, h1 the head at node 1, h2 the head at node 2, $\hat{h}$ is the interpolated head at location x.

How does this help us: we have now got a function which allows us to estimate the head at any place in the element according to the nodal values. The nodal values are only known on the boundaries, in this case at node 0, 20m and at node 5, 0m. The interpolation functions also allow us to find the rate of change, or gradient of various field parameters through differentiation. We see that equation Eq. (5.3) requires a double differential of the head to be multiplied by the permeability. A solution to equation Eq. (5.4) needs to satisfy all the physical processes, described in the flow equations, here Eq. (5.3), to give us the estimated values of the head throughout the field. Finite difference formulations work on an element by element solution of the flow equations, finite element techniques solves the flow equation globally, under the assumption that the laws governing the physical processes and the mathematical relationships remain constant throughout the area being examined. Putting this in another way, because I know the boundary conditions at nodes 0 and 5, there is a forced solution for the other nodes in the network.

Basically I translate all my physical laws into a set of ratios in my K matrix and solve for the unknown in the u and R matricis.

Galerkin is infact not a cucumber, but a very clever chap who formulated a method whereby the solutions to the equations defining the physical process being examined at every node could be combined to produce the least possible error in the overall solution of (in this case) the heads. This is known as the Galerkin method. He weights the errors coming from the application of the interpolation function at an element level providing the nodal solutions and sums over the whole network to provide the most accurate solution. The function he uses to weight the nodes is identical to the element interpretation function. To clarify this and generalising for a two nodded element i, and j

From the left hand side of the element we have

$$R_i^{(e)} = -\int_{x_i^{(e)}}^{x_j^{(e)}} N_i^{(e)} \left[K_x^{(e)} \frac{\partial^2 \hat{h}^{(e)}}{\partial x^2} \right] dx \qquad \text{Eq. (5.7)}$$

and from the right hand side of the element we have

$$R_j^{(e)} = -\int_{x_i^{(e)}}^{x_j^{(e)}} N_j^{(e)} \left[K_x^{(e)} \frac{\partial^2 \hat{h}^{(e)}}{\partial x^2} \right] dx \qquad \text{Eq. (5.8)}$$

here dx is along the length of the element. In a two dimensional element we are dealing with the surface area of the element, and a three dimensional element the volume. Fluxes are three dimensional, therefore in the FE program we multiply by a fictional area and breadth if necessary, by default 1.

Here the Ni and the Nj are the interpolation functions in the element at the nodes at that position applied to the predicted flux from the groundwater equation. Looking at an element in question, I therefore get two values of R, for the two adjacent nodes.

Example:

Using the formulation for a shape function given in Eq. (5.6)

$$\hat{h} = \frac{x_2 - x}{x_2 - x_1} h_1 + \frac{x - x_1}{x_2 - x_1} h_2$$

the element stretches from node 1 to node 2. Let us say that the value of $K_x^{(e)} \frac{\partial^2 \hat{h}^{(e)}}{\partial x^2}$ is 1 in the x direction. (How we actually get this value will be discussed later). At node 1, my value of $x=x_1$, therefore my interpolated head is after substitution:-

$$\hat{h} = \frac{x_2 - x_1}{x_2 - x_1} h_1 + \frac{x_1 - x_1}{x_2 - x_1} h_2$$
$$= 1h_1 + 0h_2$$

and likewise at node 2 my interpolated head is h_2. Now from the element perspective the flux is flowing from node 1 to node two, + into the element and – out of the element, therefore considering the "Global" matrix of residuals from this approach we get.

$$R = \begin{bmatrix} +h1 \\ -h2 \end{bmatrix} \text{ from element 1 and } R = \begin{bmatrix} +h2 \\ -h3 \end{bmatrix} \text{ from element 2} \qquad \text{Eq. (5.9)}$$

this is the fulfilment of $R_i^{(e)} = -\int_{x_i^{(e)}}^{x_j^{(e)}} N_i^{(e)} \left[K_x^{(e)} \frac{\partial^2 \hat{h}^{(e)}}{\partial x^2} \right] dx$ for node i and $R_j^{(e)} = -\int_{x_i^{(e)}}^{x_j^{(e)}} N_j^{(e)} \left[K_x^{(e)} \frac{\partial^2 \hat{h}^{(e)}}{\partial x^2} \right] dx$ for node j. The global residual matrix is then

$$R_i = \sum_e^P R_i^e \qquad \text{Eq. (5.10)}$$

6. How do we evaluate $K_x^{(e)} \frac{\partial^2 \hat{h}^{(e)}}{\partial x^2}$?

The problem we have now is that $K_x^{(e)} \frac{\partial^2 \hat{h}^{(e)}}{\partial x^2}$ includes a second order partial differential of our linear interpolation function, which isn't going to help us much here as this will equal 0. The interpolation functions do not necessarily have to be linear, but I haven't come across an example in groundwater flow where a non linear function is used. To get round this we use partial integration and apply the Gauss Greens or Gauss-Ostrogadski theorum. It seams that Gauss, Ostrogadski and Green were all involved in developing either the theory or special applications of it. Greens approach was two dimensional but equally valid in three dimensions to Gauss-Ostrogadski

Here is the simplest explanation; the mathematical description is given afterwards.

The changes in the material within an element are equal to the flux of the material through the sides of the same element.

What that means in terms of mass is I can measure the change in density in an element and multiply it by the volume of the element, i.e. integrate over the element volume, or I can describe exactly the same change by looking at the flux of matter into or out of the element. The first option is a volume integral, the second a surface integral. In the first option I have a second order partial differential equation as ($K_x^{(e)} \frac{\partial^2 \hat{h}^{(e)}}{\partial x^2}$) in a certain volume, in the second I have a gradient, grad h, multiplied by the surface area over which the flux takes place.

OK, lets look at Mr Greens[1] approach.

First Green general approach for a two dimensional plane surface:-

$$\iint_R \left(\frac{\delta g}{\delta x} - \frac{\delta f}{\delta y} \right) dxdy = \oint_c \left(f dx + g dy \right) \qquad \text{Eq. (6.1)}$$

here g and f are some function. Now substituting for groundwater flow, we want g and f to become flow functions. Ignoring permeability at this point (i.e. K=1) we get

$$\iint_R \left(\frac{\delta q_x}{\delta x} + \frac{\delta q_y}{\delta y} \right) dxdy = \oint_c (-q_y dx + q_x dy) \qquad \text{Eq. (6.2)}$$

Look at the first term in Eq. (6.2), q_x, the flux is given by $\frac{\delta h}{\delta x} K$, so by substitution we have our second order partial differential equation. On the right hand side (the signs indicate direction) we have $q_x dy$ which represents the flux through the y face in direction x. The integration along the surface c (actually a line as we are only in 2D) has a direction, at some point it is in line with the x direction, at some point it is against the x direction. This is demonstrated in Figure 6-1. On the right hand side we only have to deal with single order partial differential equations, so our linear approximation is applicable.

[1] Georg green (1793-1841), English mathematician, who was basically self educated, and the son of a baker.

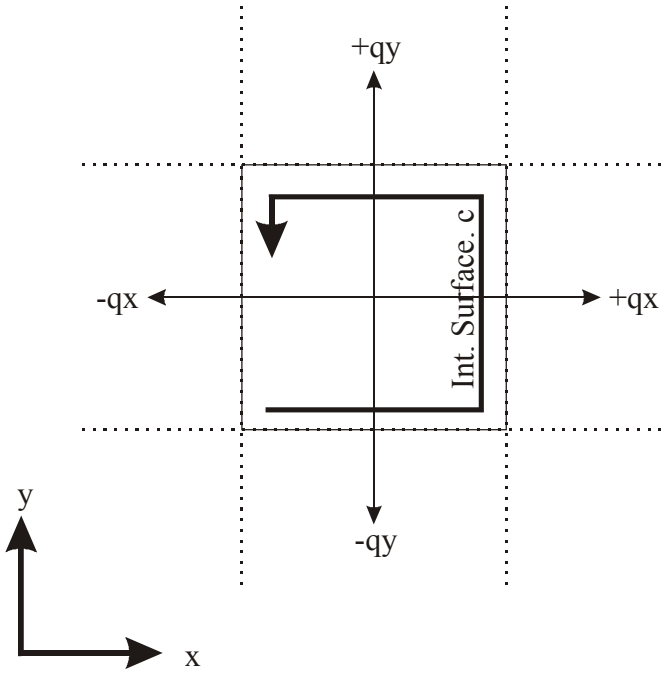


Figure 6-1: Application of Greens theorem to finite element modelling of Groundwater.

Gausses theorem is the 3D equivalent of this, i.e. volume to surface.

How is this applied in FE formulation?

Again for convenience the equation we want to solve:-

$$K_x \frac{\partial^2 h}{\partial x^2} = 0 \qquad \text{Eq. (6.3)}$$

Applying Galerkins weighting function:-

$$N_i \left(K_x \frac{\partial^2 h}{\partial x^2} \right) = 0 \qquad \text{Eq. (6.4)}$$

Rules for partial integration:

$$\phi \nabla A = \nabla (\phi A) - A \nabla \phi \qquad \text{Eq. (6.5)}$$

If we let $A = K \frac{dh}{dx}$ and $\phi = N_i$ then by substitution we can rewrite Eq. (6.4) and Eq. (6.5) as

$$N_i \nabla A = \nabla (N_i A) - A \nabla N_i \qquad \text{Eq. (6.6)}$$

Expanding this

$$\int_{x_i}^{x_j} N_i \left[K_x \frac{\partial^2 h}{\partial x^2} \right] dx = \int_{x_i}^{x_j} N_i K_x \frac{\partial \hat{h}}{\partial x} dx - \int_{x_i}^{x_j} K_x \frac{\delta N_i}{\delta x} \frac{\partial \hat{h}}{\partial x} dx \qquad \text{Eq. (6.7)}$$

Greens/Gauss/ Ostrogadski theorem is now applied to the first term, and this now becomes a flux from element to element.

$$\int_{x_i}^{x_j} N_i K_x \frac{\partial \hat{h}}{\partial x} dx = \oint_S N_i K_x \frac{\partial \hat{h}}{\partial x} ds = F_i \qquad \text{Eq. (6.8)}$$

Where S is the surface area of the element along the specified flow boundary. The sum of the flux for adjacent elements is zero, as per Eq. (5.9). At the boundaries if no flows are specified then F is zero, for elements on the boundary this term is used to specify the Neumann or specified flow rate boundary conditions.
The second term which describes the distribution of the field parameter across the mesh.

$$\int_{x_i}^{x_j} K_x \frac{\delta N_i}{\delta x} \frac{\partial \hat{h}}{\partial x} dx \qquad \text{Eq. (6.9)}$$

Both equations Eq. (6.8) and Eq. (6.9) include the term $\frac{\partial \hat{h}}{\partial x}$ which is approximated using the shape function in the element. We know $\hat{h} = \sum_i^m N_i h_i$ therefore we can substitute this term in Eq. (6.8) and Eq. (6.9). As Eq. (6.8) is either zero or specified we will ignore this term now and develop Eq. (6.9).

In our one dimensional example we have nodes i and j in the element therefore the formulation for a one dimensional bar for Eq. (6.9) is

$$\int_{x_i}^{x_j} K_x \frac{\delta N_i}{\delta x} \frac{\partial}{\partial x} \left(N_i h_i + N_j h_j \right) dx \qquad \text{Eq. (6.10)}$$

Now

$$\frac{\delta N_i}{\delta x} = \frac{\delta}{\delta x} \left(\frac{x_j - x}{x_j - x_i} \right) = -\frac{1}{x_j - x_i} = -\frac{1}{L} \qquad \text{Eq. (6.11)}$$

for $\frac{\delta N_j}{\delta x} = \frac{1}{L}$

therefore

$$\frac{\delta \hat{h}}{\delta x} = \frac{1}{L} \left(h_j - h_i \right) \qquad \text{Eq. (6.12)}$$

Substituting Eq. (6.12) into Eq. (6.10) and Eq. (6.11) into Eq. (6.10) we get for node i.

$$\begin{aligned} \int_{x_i}^{x_j} K_x \frac{\delta N_i}{\delta x} \frac{\partial}{\partial x} \left(N_i h_i + N_j h_j \right) dx &= \int_{x_i}^{x_j} K_x - \frac{1}{L} \frac{1}{L} \left(h_j - h_i \right) dx \\ &= K_x \frac{1}{L} \left(h_i - h_j \right) \end{aligned} \qquad \text{Eq. (6.13)}$$

And for the jth node we get

$$K_x \frac{1}{L} \left(-h_i + h_j \right) \qquad \text{Eq. (6.14)}$$

This can then be combined to form the matrix equation for the element:-

$$\begin{Bmatrix} R_i \\ R_j \end{Bmatrix} = \frac{K_x}{L} \begin{bmatrix} 1 & -1 \\ -1 & 1 \end{bmatrix} \begin{Bmatrix} h_i \\ h_j \end{Bmatrix} \quad \text{also } \mathbf{R} = \mathbf{Ku} \text{ for this element.} \qquad \text{Eq. (6.15)}$$

Going back a step to form a general expression and confirm where these 1's and –1's came from. Multiplying Eq. (6.10) out we get:

$$\mathbf{K} = \int_{x_i}^{x_j} K_x \begin{bmatrix} \frac{\partial N_i}{\partial x}\frac{\partial N_i}{\partial x} & \frac{\partial N_i}{\partial x}\frac{\partial N_j}{\partial x} \\ \frac{\partial N_j}{\partial x}\frac{\partial N_i}{\partial x} & \frac{\partial N_j}{\partial x}\frac{\partial N_j}{\partial x} \end{bmatrix} dx \qquad \text{Eq. (6.16)}$$

We evaluated the differential terms for the 1D case and the special shape function chosen and got to the matrix (at the element level)

$$\mathbf{K} = \frac{K_x}{L}\begin{bmatrix} 1 & -1 \\ -1 & 1 \end{bmatrix} \qquad \text{Eq. (6.17)}$$

Expanding this into three dimensions with n number of shape functions (n reflects the number of nodes in the element, that we are at the element level is noted by the symbol (e)), we get

$$R_i^{(e)} = -\iiint_{V^{(e)}} \left[K_x{}^{(e)} \frac{\partial N_i^{(e)}}{\partial x}\frac{\partial \hat{h}^{(e)}}{\partial x} + K_y{}^{(e)} \frac{\partial N_i^{(e)}}{\partial y}\frac{\partial \hat{h}^{(e)}}{\partial y} + K_z{}^{(e)} \frac{\partial N_i^{(e)}}{\partial z}\frac{\partial \hat{h}^{(e)}}{\partial z} \right] dx\,dy\,dz \quad \text{Eq. (6.18)}$$

Which then translates to

$$\underset{n\times n}{\left[K^{(e)}\right]} = \iiint_{V^{(e)}} \underset{n\times 3}{\begin{bmatrix} \frac{\partial N_1^{(e)}}{\partial x} & \frac{\partial N_1^{(e)}}{\partial y} & \frac{\partial N_1^{(e)}}{\partial z} \\ \vdots & \vdots & \vdots \\ \frac{\partial N_n^{(e)}}{\partial x} & \frac{\partial N_n^{(e)}}{\partial y} & \frac{\partial N_n^{(e)}}{\partial z} \end{bmatrix}} \underset{3\times 3}{\begin{bmatrix} K_x{}^{(e)} & 0 & 0 \\ 0 & K_y{}^{(e)} & 0 \\ 0 & 0 & K_z{}^{(e)} \end{bmatrix}} \underset{3\times n}{\begin{bmatrix} \frac{\partial N_1^{(e)}}{\partial x} & \cdots & \frac{\partial N_n^{(e)}}{\partial x} \\ \frac{\partial N_1^{(e)}}{\partial y} & \cdots & \frac{\partial N_n^{(e)}}{\partial y} \\ \frac{\partial N_1^{(e)}}{\partial z} & \cdots & \frac{\partial N_n^{(e)}}{\partial z} \end{bmatrix}} dx\,dy\,dz \quad \text{Eq. (6.19)}$$

Example

Going back to Figure 2-1 and looking at the example worksheet FE1D (Figure 6-2), and sheet "1D Dirchlet Boundaries Steady" here we set up the model, boundary conditions, and solve for the unknown heads. Remember we want to solve the equation $\mathbf{Ku} = \mathbf{R}$.

We know

$$\mathbf{u} = \begin{Bmatrix} 20 \\ h_2 \\ h_3 \\ h_4 \\ h_5 \\ 0 \end{Bmatrix} \qquad \mathbf{R} = \begin{Bmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \end{Bmatrix} \qquad \mathbf{K}\text{=6x6 matrix}$$

K is calculated as described above, and each element contribution is summed. In Figure 6-2 the geometry is indicated in the 6 rows as is the permeability of the elements. The element conductivity matrix is calculated as given above, then combined as illustrated to form a 6x6 matrix (n x n). The equation system is formed and now the boundary conditions must be addressed. Where the head is already specified then we do not need to solve for the head in the equations, rather we need to eliminate these rows from the matrix formulation. An example of an elimination is given in Figure 6-3.

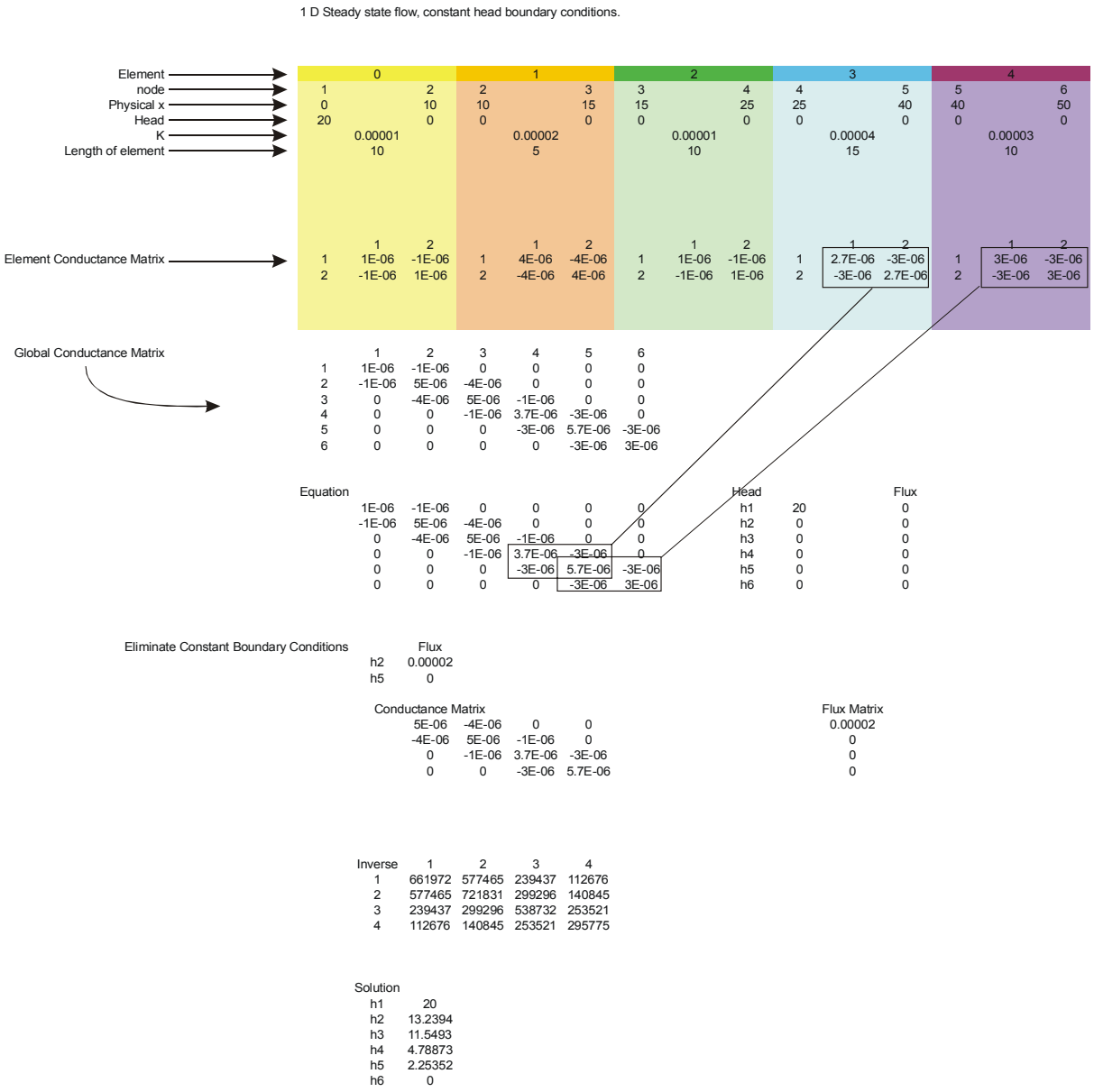


Figure 6-2: Example of the solution of a 1D FE problem in GW flow using excel. Steady state conditions and constant head (Dirchlet) boundary conditions.

The conductance matrix is then reformed, in this case the inverse of the matrix is calculated, and the values of h2,h3,h4and h5 calculated.

	1	2	3	4	5	6	Heads		R
1	a1	a2	a3	a4	a5	a6	20		0
2	b1	b2	b3	b4	b5	b6	h2		0
3	c1	c2	c3	c4	c5	c6	h3	=	0
4	d1	d2	d3	d4	d5	d6	h4		0
5	e1	e2	e3	e4	e5	e6	h5		0
6	f1	f2	f3	f4	f5	f6	0		0

20b1+h2b2+h3b3+h4b4+h5b5+h6b6=0
20c1+h2c2+h3c3+h4c4+h5c5+h6c6=0
20d1+h2d2+h3d3+h4d4+h5d5+h6d6=0
20e1+h2e2+h3e3+h4e4+h5e5+h6e6=0

Therefore we can replace h2 and eliminate the top row as follows

h2b2+h3b3+h4b4+h5b5=-20b1-h6b6
h2c2+h3c3+h4c4+h5c5=-20c1-h6c6
h2d2+h3d3+h4d4+h5d5=-20d1-h6d6
h2e2+h3e3+h4e4+h5e5=-20e1-h6e6

Figure 6-3: Dealing with boundary conditions.

7. Inclusion of a source term (e.g. a well pumping water into the system).

A source term may be added by including a value in the flux vector. An example of this is given in

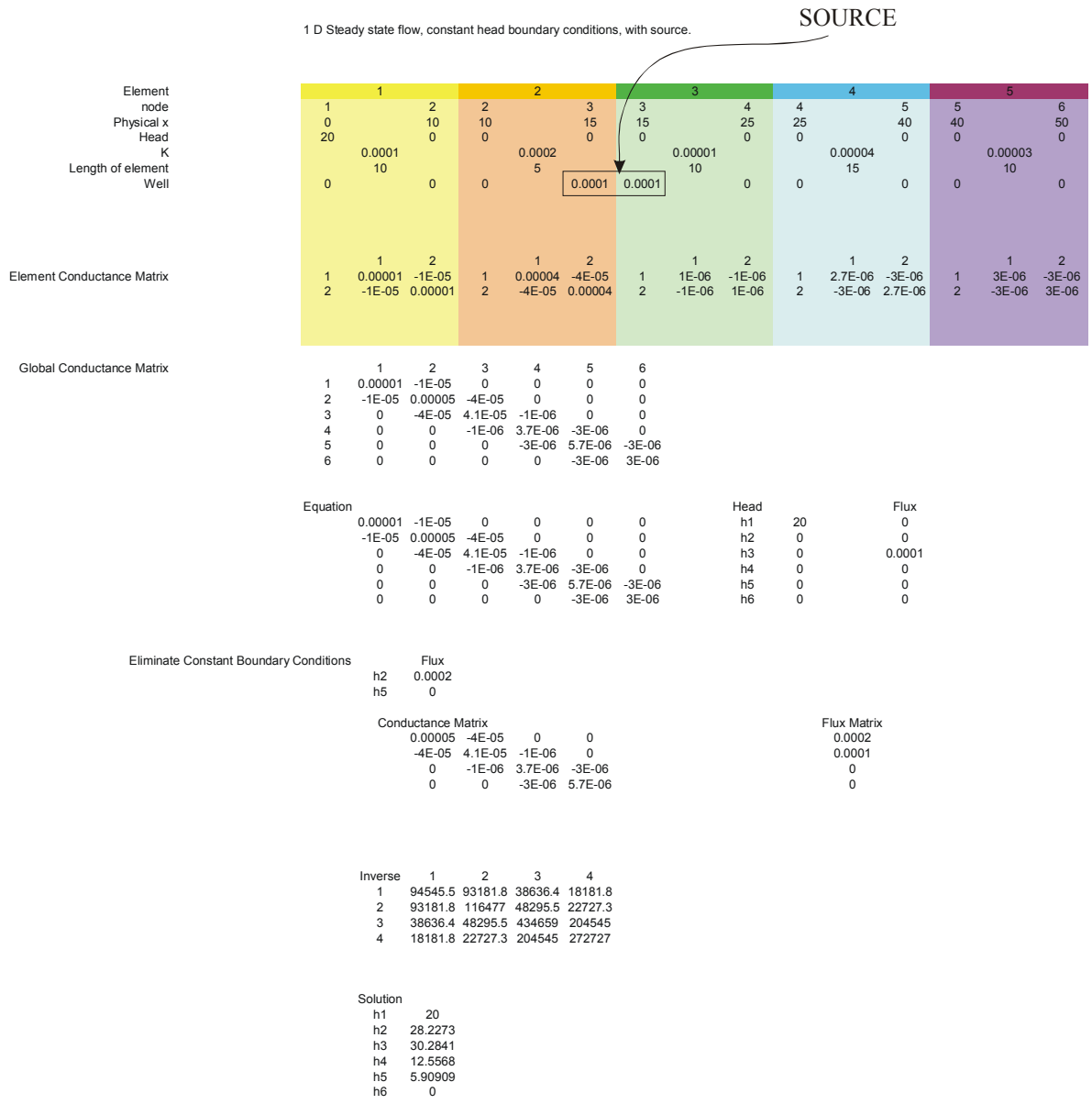


Figure 7-1: Example of 1D FE model with a source at node 3.

8. Inclusion of Storage (Transient Flow Conditions).

Under transient flow conditions water doesn't just flow through the material, it also either fills it up abit or drains it. For a certain pressure difference, given as equivalent to a 1m head change, a certain amount of water can go into or out of storage. This is known as transient flow, or unsteady state flow. After a certain amount of time no more water goes into the material through whcih it is flowing, and we get steady state flow conditions. This is represented by the equation

$$\frac{\partial}{\partial x}\left(K_x \frac{\partial h}{\partial x}\right)+\frac{\partial}{\partial y}\left(K_y \frac{\partial h}{\partial y}\right)+\frac{\partial}{\partial z}\left(K_z \frac{\partial h}{\partial z}\right)=S_s \frac{\partial h}{\partial t} \qquad \text{Eq. (8.1)}$$

here we have S_s as a constant and the flux into and out of storage as dependent on the rate of change of head with time.

How do we include storage in the FE model?.

The groundwater equation is expressed as

$$R_i^{(e)} = -\iiint_{V^{(e)}} N_i^{(e)} \left[K_x^{(e)} \frac{\partial^2 \hat{h}^{(e)}}{\partial x^2} + K_y^{(e)} \frac{\partial^2 \hat{h}^{(e)}}{\partial y^2} + K_z^{(e)} \frac{\partial^2 \hat{h}^{(e)}}{\partial z^2} - S_s^{(e)} \frac{\partial \hat{h}^{(e)}}{\partial t} \right] dx\, dy\, dz \qquad \text{Eq. (8.2)}$$

In matrix terms we now write

$$\mathbf{R} = \mathbf{K}\mathbf{u} + \mathbf{C}\dot{\mathbf{u}} \qquad \text{Eq. (8.3)}$$

where $\dot{\mathbf{u}}$ represents the time differential of the heads.

Looking at this equation we will derive the various parts bit by bit. What happens to the terms involving $\frac{\partial^2 \hat{h}^{(e)}}{\partial x^2}$ has been covered in the previous section. Now we need to consider on the term $S_s^{(e)} \frac{\partial \hat{h}^{(e)}}{\partial t}$. Here we develop the **Capacitance Matrix (C)**.

Capacitance Matrix (C).
The value of R should be zero, therefore there is a contribution from both the Conductance (K) and Capacitance (C) matrix.

$$\begin{Bmatrix} R_1 \\ \vdots \\ R_n \end{Bmatrix}_K = K \begin{Bmatrix} h_1 \\ \vdots \\ h_n \end{Bmatrix} \quad \text{and} \quad \begin{Bmatrix} R_1 \\ \vdots \\ R_n \end{Bmatrix}_C = C \begin{Bmatrix} \frac{\partial h_1}{\partial t} \\ \vdots \\ \frac{\partial h_n}{\partial t} \end{Bmatrix} \qquad \text{Eq. (8.4)}$$

Ignoring other terms and multiplying Eq. (8.2) out we have for the one dimensional case:-

$$\int_V N_i S_s (N_i \frac{\partial h_i}{\partial t} + N_j \frac{\partial h_j}{\partial t}) dx \qquad \text{Eq. (8.5)}$$

For the three dimensional case we have:-

$$\underset{n\times n}{\left[C^{(e)}\right]}=\iiint_{V^{(e)}}\begin{bmatrix}N_1^{(e)}\\ \vdots \\ N_n^{(e)}\end{bmatrix}_{n\times 1}\left[S_s^{(e)}\right]_{1\times 1}\underset{1\times n}{\left[N_1^{(e)}\cdots N_n^{(e)}\right]}dx\,dy\,dz \qquad \text{Eq. (8.6)}$$

Consider now Eq. (8.5), and the element matrix it should develop.

The functions Ni and Nj are

$$N_i=\frac{x_j-x}{x_j-x_i}$$
$$N_j=\frac{x-x_i}{x_j-x_i} \qquad \text{Eq. (8.7)}$$

Calculating the first entrance in this matrix we have

$$\int_{x_i}^{x_j}\frac{x_j-x}{x_j-x_i}\times\frac{x-x_i}{x_j-x_i}dx \qquad \text{Eq. (8.8)}$$

Here the maths program MAPEL helps in the evaluation, x_i is substituted with a and x_j with b for clarity:

$$f:=\frac{(b-x)(x-a)}{(b-a)^2}$$

$$-\frac{1}{3}\frac{b^3-a^3}{(b-a)^2}+\frac{1}{2}\left(\frac{b}{(b-a)^2}+\frac{a}{(b-a)^2}\right)(b^2-a^2)-\frac{b\,a}{b-a}$$

```
> a:=0;
```
$a := 0$

```
> b:=1;
```
$b := 1$

```
> f:=((b-x)/(b-a))*((b-x)/(b-a));
```
$f := (1-x)^2$

```
> int(f, x=a..b);
```
$\frac{1}{3}$

```
> f:=((b-x)/(b-a))*((x-a)/(b-a));
```
$f := (1-x)\,x$

```
> int(f, x=a..b);
```

$\frac{1}{6}$

Note that this element stretches from x=0 to x=1, i.e. a unit element. (Later we will use local coordinate systems from –1 to +1, below is valid except it would be multiplied by $\frac{1}{3}$).

$$\int_V \begin{bmatrix} N_i N_i & N_i N_j \\ N_j N_i & N_j N_j \end{bmatrix} dx = \frac{1}{6}\begin{bmatrix} 2 & 1 \\ 1 & 2 \end{bmatrix} \qquad \text{Eq. (8.9)}$$

If the coordinates are different the same local element solution can be used but transformed into real coordinates. The total sum of contribution of S to the entire area of the finite element is 1.

The above method is the Consistent Formulation approach.

A second method is called the Lumped Element Formulation. In the lumped the contribution of the storage in the element is divided by the number of nodes in the element. A different interpolation function is used than for the head distribution. The formulation becomes

$$C^{(e)} = S_s^{(e)} \frac{V^{(e)}}{n} \begin{bmatrix} 1 & & 0 \\ & \ddots & \\ 0 & & 1 \end{bmatrix}_{nxn} \qquad \text{Eq. (8.10)}$$

Where n represents the number of nodes.

The lumped element formulation is less accurate than the consistent element formulation but provides easier solutions and saves time. Both options can be selected in Rockflow, and the final result is almost identical. The global capacitance matrix is formed in the same way as the global conductance matrix, with the addition of terms applicable to the various elements.

Treatment of $\dot{\mathbf{u}}$.

The values in $\dot{\mathbf{u}}$ are estimated by taking the known, or calculated values of h and defining the differential $\frac{dh}{dt} = \frac{h(t+\Delta t)}{\Delta t}$ where Δt is given either by the user or calculated.

Following Istok (1989) exactly, Figure 8-1 illustrates a variable ε which is a measure of what

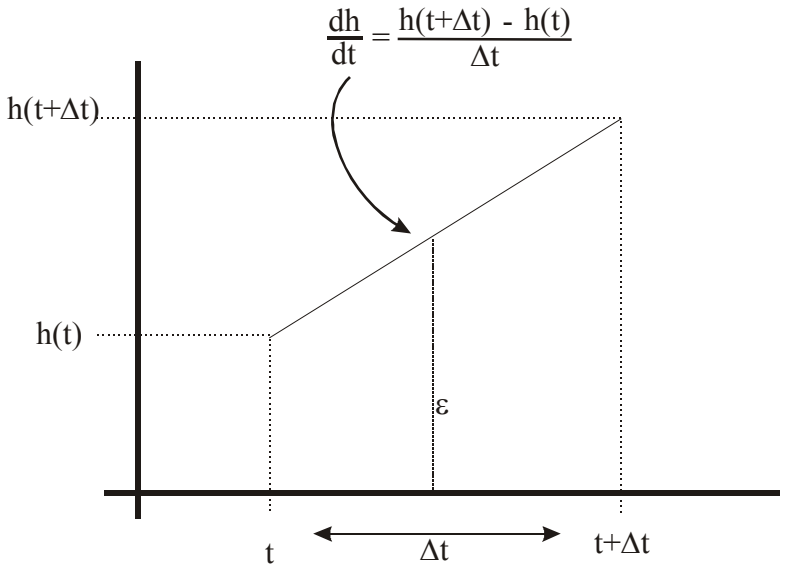


Figure 8-1: Time derivate of hydraulic head

Position along the gradient of the interval t to Δt is taken for the analysis. ε is replaced by a variable ω, defined as :

$$\varpi = \frac{\varepsilon - t}{\Delta t} \qquad \text{Eq. (8.11)}$$

that is ω represents how far towards the new solutions of h we are.

There are three main subsets of solutions the time derivation:-

ω=0, Forward Difference Method

$$[C]\{h\}_{t+\Delta t} = \left([C] - \Delta t[K]\right)\{h\}_t + \frac{\Delta t}{2} R_{t+\Delta t} \qquad \text{Eq. (8.12)}$$

ω =0.5, Central Difference Method

$$\left([C] + \frac{\Delta t}{2}[K]\right)\{h\}_{t+\Delta t} = \left([C] - \frac{\Delta t}{2}[K]\right)\{h\}_t + \frac{\Delta t}{2}\left(R_t + R_{t+\Delta t}\right) \qquad \text{Eq. (8.13)}$$

ω =1, Backward Difference Method.

$$\left([C] + \Delta t[K]\right)\{h\}_{t+\Delta t} = [C]\{h\}_t + \Delta t R_{t+\Delta t} \qquad \text{Eq. (8.14)}$$

As an example let us define the unknown hydraulic heads in the Crank-Nicholson Method

$$\{h\} = \frac{1}{2}h(t) + \frac{1}{2}h(t+\Delta t) \qquad \text{Eq. (8.15)}$$

This is all summed up in the finite difference formulation

$$\left([C] + \varpi\Delta t[K]\right)\{h\}_{t+\Delta t} = \left([C] - (1-\varpi)\Delta t[K]\right)\{h\}_t + \Delta t\left((1-\varpi)\{R\}_t + \varpi\{R\}_{t+\Delta t}\right) \text{ Eq. (8.16)}$$

Going back to Eq. (8.3), we can now solve for the new time steps heads, as all the heads in the previous time step are known.

An example of a 1D model including storage is presented in Figure 8-2 for a backward difference Eq. (8.14) approach. This is included under the worksheet 1D Dirchlet Transient.

Two time steps.

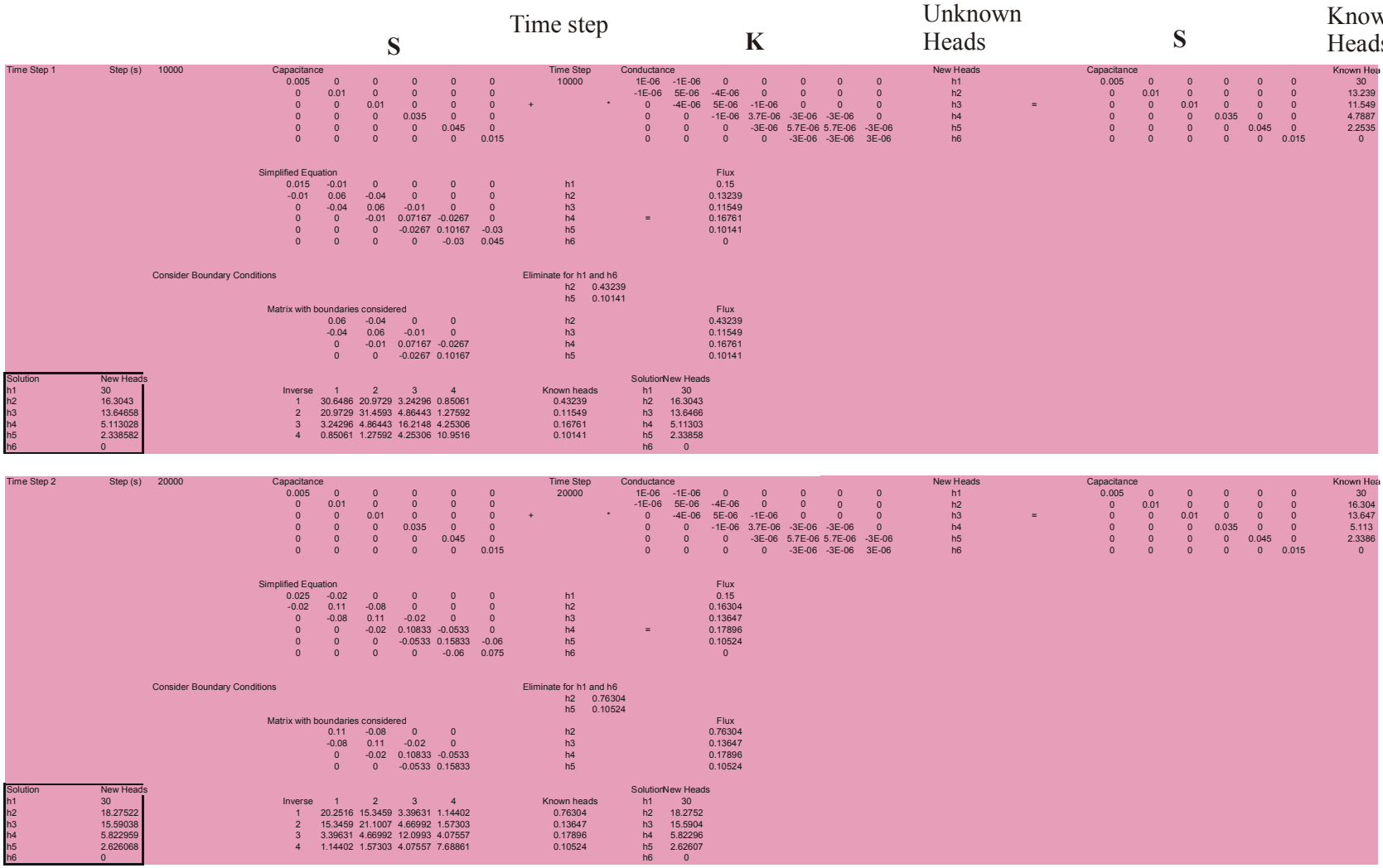


Figure 8-2: Worksheet, transient groundwater flow, 1D model, Dirchlet boundary Conditions.

9. Solute Transport Finite Element Formulation.

Here we include a coupled process. The solution of the solute transport process is dependent upon first the solution of the groundwater flow to give us groundwater velocities, from which we can then solve the solute equation. The coupling term is then the groundwater velocity in the elements. In practise we solve first the groundwater flow for the first time step, then recover the velocities for each element from the head differences, permeability and porosity, then move to the transport terms.

The solute transport equation looks quite horrible, and it is quite horrible!, but if you fight with it you will get on top of it.

$$\begin{aligned}\frac{\partial(\theta C)}{\partial t} &= D_x\frac{\partial^2}{\partial x^2}(\theta C) + D_y\frac{\partial^2}{\partial y^2}(\theta C) + D_z\frac{\partial^2}{\partial z^2}(\theta C)\\ &\quad -\frac{\partial}{\partial x}(v_x C) - \frac{\partial}{\partial y}(v_y C) - \frac{\partial}{\partial z}(v_z C) - \frac{\partial}{\partial t}(\rho_b K_d C)\\ &\quad -\lambda(\theta C + \rho_b K_d C)\end{aligned} \qquad \text{Eq. (9.1)}$$

Which in finite element formulation can be written

$$\begin{aligned}R_i^{(e)} = -\iiint_{V^{(e)}} N_i^{(e)}(x,y,z)\Bigg[& D_x{}^{(e)}\theta^{(e)}\frac{\partial^2\hat{C}^{(e)}}{\partial x^2} + D_y{}^{(e)}\theta^{(e)}\frac{\partial^2\hat{C}^{(e)}}{\partial y^2} + D_z{}^{(e)}\theta^{(e)}\frac{\partial^2\hat{C}^{(e)}}{\partial z^2}\\ & -v_x{}^{(e)}\frac{\partial\hat{C}^{(e)}}{\partial x} - v_y\frac{\partial C}{\partial y} - v_z\frac{\partial C}{\partial z}\\ & -\rho_b{}^{(e)}K_d{}^{(e)}\frac{\partial\hat{C}^{(e)}}{\partial t} - \lambda\left(\theta^{(e)}\hat{C}^{(e)} + \rho_b{}^{(e)}K_d{}^{(e)}\hat{C}^{(e)}\right) - \frac{\partial}{\partial t}\left(\theta^{(e)}\hat{C}^{(e)}\right)\Bigg]dx\,dy\,dz\end{aligned} \qquad \text{Eq. (9.2)}$$

This is rewritten as

$$\mathbf{R} = \mathbf{DC} + \mathbf{A}\dot{\mathbf{C}} \qquad \text{Eq. (9.3)}$$

Here R is the residual again, **D** is the advection dispersion matrix, **A** is the element sorption matrix and **C** is the concentration $\dot{\mathbf{C}}$ is the rate of change of concentration with time. Looking at the terms in Eq. (9.4) we see that we can combine a number in **D** and a number in **A**, to give us Eq. (9.3).

$$R_i^{(e)} = -\iiint_{V^{(e)}} N_i^{(e)} \left[D_x{}^{(e)}\theta^{(e)} \frac{\partial^2 \hat{C}^{(e)}}{\partial x^2} + D_y{}^{(e)}\theta^{(e)} \frac{\partial^2 \hat{C}^{(e)}}{\partial y^2} + D_z{}^{(e)}\theta^{(e)} \frac{\partial^2 \hat{C}^{(e)}}{\partial z^2} \right] dx\,dy\,dz$$ Diff. and disp terms.

$$+\iiint_{V^{(e)}} N_i^{(e)} \left[v_x{}^{(e)} \frac{\partial \hat{C}^{(e)}}{\partial x} - v_y \frac{\partial C}{\partial y} - v_z \frac{\partial C}{\partial z} \right] dx\,dy\,dz$$ Advection terms.

$$+\iiint_{V^{(e)}} N_i^{(e)} \left[\rho_b{}^{(e)} K_d{}^{(e)} \frac{\partial \hat{C}^{(e)}}{\partial t} \right] dx\,dy\,dz$$ Sorbtion on solid term.

$$+\iiint_{V^{(e)}} N_i^{(e)} \left[\lambda \left(\theta^{(e)} \hat{C}^{(e)} + \rho_b{}^{(e)} K_d{}^{(e)} \hat{C}^{(e)} \right) \right] dx\,dy\,dz$$ Solute decay in solvent and on solid.

$$+\iiint_{V^{(e)}} N_i^{(e)} \left[\frac{\partial}{\partial t} \left(\theta^{(e)} \hat{C}^{(e)} \right) \right] dx\,dy\,dz$$ Change in concentration in solvent with time.

Eq. (9.4)

D is formulated now as

$$\mathbf{D} = \iiint_{v^{(e)}} \begin{bmatrix} \frac{\delta N_1}{\delta x} & \frac{\delta N_1}{\delta y} & \frac{\delta N_1}{\delta z} \\ \vdots & \vdots & \vdots \\ \frac{\delta Nn}{\delta x} & \frac{\delta Nn}{\delta y} & \frac{\delta Nn}{\delta z} \end{bmatrix} \begin{bmatrix} D_{xx}^{(e)}\theta(t) & D_{xy}^{(e)}\theta(t) & D_{xz}^{(e)}\theta(t) \\ D_{yx}^{(e)}\theta(t) & D_{yy}^{(e)}\theta(t) & D_{yz}^{(e)}\theta(t) \\ D_{zx}^{(e)}\theta(t) & D_{zy}^{(e)}\theta(t) & D_{zz}^{(e)}\theta(t) \end{bmatrix} \begin{bmatrix} \frac{\delta N_1}{\delta x} & \cdots & \frac{\delta Nn}{\delta x} \\ \frac{\delta N_1}{\delta y} & \cdots & \frac{\delta Nn}{\delta y} \\ \frac{\delta N_1}{\delta z} & \cdots & \frac{\delta Nn}{\delta z} \end{bmatrix} dxdydz$$

$$+\iiint_{v^{(e)}} \begin{bmatrix} N_1^{(e)} & N_1^{(e)} & N_1^{(e)} \\ \vdots & \vdots & \vdots \\ N_n^{(e)} & N_n^{(e)} & N_n^{(e)} \end{bmatrix} \begin{bmatrix} v_x^{(e)}t & 0 & 0 \\ 0 & v_y^{(e)}t & 0 \\ 0 & 0 & v_z^{(e)}t \end{bmatrix} \begin{bmatrix} \frac{\delta N_1}{\delta x} & \cdots & \frac{\delta Nn}{\delta x} \\ \frac{\delta N_1}{\delta y} & \cdots & \frac{\delta Nn}{\delta y} \\ \frac{\delta N_1}{\delta z} & \cdots & \frac{\delta Nn}{\delta z} \end{bmatrix} dxdydz$$ Eq. (9.5)

$$+\iiint_{v^{(e)}} \begin{bmatrix} N_1^{(e)} \\ \vdots \\ N_n^{(e)} \end{bmatrix} \left[\lambda \left(\theta^{(e)} \hat{C}^{(e)} + \rho_b{}^{(e)} K_d{}^{(e)} \hat{C}^{(e)} \right) \right] \left[N_1^{(e)} \cdots N_n^{(e)} \right] dxdydz$$

A is given by

$$\left[\mathbf{A}^{(e)}(t) \right] = \iiint_{v^{(e)}} \begin{bmatrix} N_1^{(e)} \\ \vdots \\ N_n^{(e)} \end{bmatrix} \left[\rho_b{}^{(e)} K_d{}^{(e)} + \theta^{(e)}(t) \right] \left[N_1^{(e)} \quad \cdots \quad N_n^{(e)} \right] dx\,dy\,dz$$ Eq. (9.6)

This is now solved as

$$\left(\left[A(t+\Delta t) \right] + \varpi \Delta t \left[D(t+\Delta t) \right] \right) \{C\}_{t+\Delta t} = \left(A(t) - (1-\varpi)\Delta t \left[D(t) \right] \right) \{C\}_t + \Delta t \left((1-\varpi) \{R\}_t + \varpi \{R\}_{t+\Delta t} \right)$$

Eq. (9.7)

An example of a backward difference scheme for the one dimensional case solved for groundwater flow is illustrated in Figure 9-1 (also in excel sheet). To solve this equation first the groundwater problem is solved to obtain values dependent on the groundwater flow characteristics for the first chosen time step. Then the initial values of $\{C\}_t$ are specified and the various matrices are calculated to allow us to solve for $\{C\}_{t+\Delta t}$ at the end of the time step. The values of $\{C\}_{t+\Delta t}$ are then used to define $A(t+\Delta t)$ and $D(t+\Delta t)$ and the solution procedure is repeated iteratively.

This procedure is valid when changes in the density due to changes in the solute concentration in the aquifer are assumed to be negligibly small. If this is not true then the groundwater and solute transport equations need to be solved simultaneously.

1 D steady flow with transport, constant head

Element		1			2			3			4			5	
node		1		2	2		3	3		4	4		5	5		6
Physical x		0		10	10		15	15		25	25		40	40		50
Head from example 1		20		13.2394	13.2394		11.5493	11.5493		4.78873	4.78873		2.25352	2.25352		0
K			0.00001			0.00002			0.00001			0.00004			0.00003	
S			0.001			0.002			0.001			0.004			0.003	
Velocity (m/s)			6.8E-06			6.8E-06			6.8E-06			6.8E-06			6.8E-06	
n			0.2			0.2			0.2			0.2			0.2	
Length of element			10			5			10			15			10	
C(t=0)		50		0	0		0	0		0	0		0	0		0
Dx (m²/s)	1.00E-05															

Element Dispersion Matrix		1	2		1	2		1	2		1	2		1	2
	1	1E-06	-1E-06	1	2E-06	-2E-06	1	1E-06	-1E-06	1	6.7E-07	-7E-07	1	1E-06	-1E-06
	2	-1E-06	1E-06	2	-2E-06	2E-06	2	-1E-06	1E-06	2	-7E-07	6.7E-07	2	-1E-06	1E-06

Element Advective Matrix		1	2		1	2		1	2		1	2		1	2
	1	-2E-05	1.7E-05	1	-2E-05	1.7E-05	1	-2E-05	1.7E-05	1	-2E-05	1.7E-05	1	-2E-05	1.7E-05
	2	-2E-05	1.7E-05	2	-2E-05	1.7E-05	2	-2E-05	1.7E-05	2	-2E-05	1.7E-05	2	-2E-05	1.7E-05

Element Advective Dispersion Matrix		1	2		1	2		1	2		1	2		1	2
	1	-2E-05	1.6E-05	1	-1E-05	1.5E-05	1	-2E-05	1.6E-05	1	-2E-05	1.6E-05	1	-2E-05	1.6E-05
	2	-2E-05	1.8E-05	2	-2E-05	1.9E-05	2	-2E-05	1.8E-05	2	-2E-05	1.8E-05	2	-2E-05	1.8E-05

Element Sorption Matrix		1	2		1	2		1	2		1	2		1	2
	1	5	0	1	2.5	0	1	5	0	1	7.5	0	1	5	0
	2	0	5	2	0	2.5	2	0	5	2	0	7.5	2	0	5

Global Dispersion Advective Matrix

j/i	1	2	3	4	5	6
1	-2E-05	1.6E-05	0	0	0	0
2	-2E-05	3E-06	1.5E-05	0	0	0
3	0	-2E-05	3E-06	1.6E-05	0	0
4	0	0	-2E-05	1.7E-06	1.6E-05	0
5	0	0	0	-2E-05	1.7E-06	1.6E-05
6	0	0	0	0	-2E-05	1.8E-05

Global Sorption Matrix

j/i	1	2	3	4	5	6
1	5	0	0	0	0	0
2	0	7.5	0	0	0	0
3	0	0	7.5	0	0	0
4	0	0	0	12.5	0	0
5	0	0	0	0	12.5	0
6	0	0	0	0	0	5

Time step 432000 Flux Vector / Known Solute Concentrations

1	0	C1	50	
2	0	C2	0	
3	0	C3	0	
4	0	C4	0	
5	0	C5	0	
6	0	C6	0	

j/i	1	2	3	4	5	6			
1	-1.8694	6.86941	0	0	0	0	C1		250
2	-7.7334	8.796	6.43741	0	0	0	C2	=	0
3	0	-8.1654	8.796	6.86941	0	0	C3		0
4	0	0	-7.7334	13.22	7.01341	0	C4		0
5	0	0	0	-7.5894	13.22	6.86941	C5		0
6	0	0	0	0	-7.7334	12.7334	C6		0

Time step 432000 Flux Vector / Known Solute Concentrations

1	0	C1	50	
2	0	C2	0	
3	0	C3	0	
4	0	C4	0	
5	0	C5	0	
6	0	C6	0	

j/i	1	2	3	4	5	6			
1	-1.8694	6.86941	0	0	0	0	C1		250
2	-7.7334	8.796	6.43741	0	0	0	C2	=	0
3	0	-8.1654	8.796	6.86941	0	0	C3		0
4	0	0	-7.7334	13.22	7.01341	0	C4		0
5	0	0	0	-7.5894	13.22	6.86941	C5		0
6	0	0	0	0	-7.7334	12.7334	C6		0

Boundary Conditions..eliminating C1

Flux

C2	386.67

Matrix

8.796	6.43741	0	0	0	C2		386.67
-8.1654	8.796	6.86941	0	0	C3	=	0
0	-7.7334	13.22	7.01341	0	C4		0
0	0	-7.5894	13.22	6.86941	C5		0
0	0	0	-7.7334	12.7334	C6		0

Inverse	1	2	3	4	5	Concentration Values
1	0.07602	-0.0406	0.01712	-0.0069	0.00372	29.3937
2	0.05147	0.05545	-0.0234	0.00943	-0.0051	19.903
3	0.02445	0.02634	0.05031	-0.0203	0.01094	9.45416
4	0.01067	0.01149	0.02195	0.04864	-0.0262	4.12554
5	0.00648	0.00698	0.01333	0.02954	0.0626	2.50557

Concentration Profile after timestep

C1	50
C2	29.3937
C3	19.903
C4	9.45416
C5	4.12554
C6	2.50557

Figure 9-1: Spread of contamination in a one dimensional aquifer model. One time step.

10. Heat Transport

The solution of the heat transport equation follows that of solute transport very closely.

The heat transport equation is given as

$$\begin{aligned} c\rho\frac{\partial T}{\partial t} &= D_x\frac{\partial^2 T}{\partial x^2} + D_y\frac{\partial^2 T}{\partial y^2} + D_z\frac{\partial^2 T}{\partial z^2} \\ &\quad - c^w\rho^w v_x\frac{\partial T}{\partial x} - c^w\rho^w v_y\frac{\partial T}{\partial y} - c^w\rho^w v_z\frac{\partial T}{\partial z} \\ &\quad - \rho Q_T \end{aligned} \tag{10.1}$$

Here the heat diffusion dispersion tensor contains a component for diffusion, and a component for dispersion due to advection

$$D_\gamma = D_e + v_\gamma\beta \tag{10.2}$$

where D_γ is the heat diffusion dispersion coefficient in the γ direction (kJ°C^{-1} m^{-1} s^{-1}), D_e is the effective heat diffusion coefficient (kJ°C^{-1} m^{-1} s^{-1}) (de Marsily (1986)) comprising a combination of the rock and fluid heat diffusion coefficients.

$$D_e = nD^w + (1-n)D^r \tag{10.3}$$

Further v_γ is the advective flow velocity in the α direction (m/s) and β is the heat dispersion coefficient (kJ°C^{-1} m^{-2}). β can be broken down into the mechanical dispersion α as seen in solute transport and the heat energy properties of the material.

$$\beta = \alpha_l\rho c^w \tag{10.4}$$

Equivalent to the Darcy equation heat transport can be expressed as energy moving along a heat gradient.

$$q = -\mathrm{K}\frac{dT}{dx} \tag{10.5}$$

where q is the heat flux in Watts per m² (W/m²), and K is the thermal conductivity in J/m.s.K. There is a relationship between the heat dispersion coefficient and the thermal conductivity such that

$$D = \frac{\mathrm{K}}{\rho c_p} \tag{10.6}$$

Expressing this as per the solute equation previously in finite element formulation:

$$
\begin{aligned}
R_i^{(e)} = &-\iiint_{V^{(e)}} N_i^{(e)} \left[D_x{}^{(e)} \frac{\partial^2 \hat{T}^{(e)}}{\partial x^2} + D_y{}^{(e)} \frac{\partial^2 \hat{T}^{(e)}}{\partial y^2} + D_z{}^{(e)} \frac{\partial^2 \hat{T}^{(e)}}{\partial z^2} \right] dx\,dy\,dz \quad \text{Conduction} \\
&+ \iiint_{V^{(e)}} N_i^{(e)} \left[v_x{}^{(e)} \rho^w c^w \frac{\partial \hat{T}^{(e)}}{\partial x} - v_y \rho^w c^w \frac{\partial \hat{T}^{(e)}}{\partial y} - v_z \rho^w c^w \frac{\partial \hat{T}^{(e)}}{\partial z} \right] dx\,dy\,dz \quad \text{Convection} \\
&+ \iiint_{V^{(e)}} N_i^{(e)} \left[\rho Q_T \right] dx\,dy\,dz \qquad\qquad \text{Source} \\
&+ \iiint_{V^{(e)}} N_i^{(e)} \left[\rho c \frac{\partial T}{\partial t} \right] dx\,dy\,dz \qquad\qquad \text{Change in temperature with time.}
\end{aligned}
\tag{10.7}
$$

ρc refers to the combined density and heat capacity of the solid and fluid in an element.

The conduction convection matrix can be formulated as

$$
\begin{aligned}
\mathbf{D} = &\iiint_{v^{(e)}} \begin{bmatrix} \frac{\delta N_1}{\delta x} & \frac{\delta N_1}{\delta y} & \frac{\delta N_1}{\delta z} \\ \vdots & \vdots & \vdots \\ \frac{\delta Nn}{\delta x} & \frac{\delta Nn}{\delta y} & \frac{\delta Nn}{\delta z} \end{bmatrix} \begin{bmatrix} D_{xx}^{(e)}\theta(t) & D_{xy}^{(e)}\theta(t) & D_{xz}^{(e)}\theta(t) \\ D_{yx}^{(e)}\theta(t) & D_{yy}^{(e)}\theta(t) & D_{yz}^{(e)}\theta(t) \\ D_{zx}^{(e)}\theta(t) & D_{zy}^{(e)}\theta(t) & D_{zz}^{(e)}\theta(t) \end{bmatrix} \begin{bmatrix} \frac{\delta N_1}{\delta x} & \cdots & \frac{\delta Nn}{\delta x} \\ \frac{\delta N_1}{\delta y} & \cdots & \frac{\delta Nn}{\delta y} \\ \frac{\delta N_1}{\delta z} & \cdots & \frac{\delta Nn}{\delta z} \end{bmatrix} dxdydz \\
&+ \iiint_{v^{(e)}} \begin{bmatrix} N_1^{(e)} & N_1^{(e)} & N_1^{(e)} \\ \vdots & \vdots & \vdots \\ N_n^{(e)} & N_n^{(e)} & N_n^{(e)} \end{bmatrix} \begin{bmatrix} v_x^{(e)} \rho^w c^w(t) & 0 & 0 \\ 0 & v_y^{(e)} \rho^w c^w(t) & 0 \\ 0 & 0 & v_z^{(e)} \rho^w c^w(t) \end{bmatrix} \begin{bmatrix} \frac{\delta N_1}{\delta x} & \cdots & \frac{\delta Nn}{\delta x} \\ \frac{\delta N_1}{\delta y} & \cdots & \frac{\delta Nn}{\delta y} \\ \frac{\delta N_1}{\delta z} & \cdots & \frac{\delta Nn}{\delta z} \end{bmatrix} dxdydz
\end{aligned}
\tag{10.8}
$$

$$
\left[\mathbf{A}^{(e)}(t) \right] = \iiint_{v^{(e)}} \begin{bmatrix} N_1^{(e)} \\ \vdots \\ N_n^{(e)} \end{bmatrix} [c\rho] \begin{bmatrix} N_1^{(e)} & \cdots & N_n^{(e)} \end{bmatrix} dx\,dy\,dz \tag{10.9}
$$

The source term can be included in the flux matrix **R** so we can express the heat transport problem in matrix form as

$$
\mathbf{R} = \mathbf{DT} + \mathbf{A}\dot{\mathbf{T}} \tag{10.10}
$$

11. Stress Strain Analysis

The approach is similar to the groundwater approach, as would be expected the formulation of the problem is different.

The basis of the assessment of stress and strain in the finite element approach is the consideration of the stress equilibrium in the body being investigated. After Jaeger and Cook (1976, p. 116-118)the equilibrium equations can be written as

$$\frac{\delta T_{xx}}{\delta x}+\frac{\delta T_{xy}}{\delta y}+\frac{\delta T_{xz}}{\delta z}+\frac{d\sigma_{xx}}{dx}+\frac{d\sigma_{xy}}{dy}+\frac{d\sigma_{xz}}{dz}+\rho B_x=0 \qquad \text{Eq. (11.1)}$$

$$\frac{\delta T_{yx}}{\delta x}+\frac{\delta T_{yy}}{\delta y}+\frac{\delta T_{yz}}{\delta z}+\frac{d\sigma_{yx}}{dx}+\frac{d\sigma_{yy}}{dy}+\frac{d\sigma_{yz}}{dz}+\rho B_y=0 \qquad \text{Eq. (11.2)}$$

$$\frac{\delta T_{zx}}{\delta x}+\frac{\delta T_{zy}}{\delta y}+\frac{\delta T_{zz}}{\delta z}+\frac{d\sigma_{zx}}{dx}+\frac{d\sigma_{zy}}{dy}+\frac{d\sigma_{zz}}{dz}+\rho B_z=0 \qquad \text{Eq. (11.3)}$$

The initial stress, sometime known as thermal stress, or maybe tectonic stress is in the stress tensor T. The applied stress is in the stress tensor σ. B represents body forces, such as electrostatic forces or gravity. If gravity then $\rho B_z = \rho g$.

Strain is related to stress, here over linear elasticity.

$$\begin{bmatrix}\varepsilon_{xx}\\ \varepsilon_{yy}\\ \varepsilon_{zz}\\ \varepsilon_{xy}\\ \varepsilon_{yz}\\ \varepsilon_{xy}\end{bmatrix}=\frac{1}{E}\begin{bmatrix}1 & -v & -v & 0 & 0 & 0\\ -v & 1 & -v & 0 & 0 & 0\\ -v & -v & 1 & 0 & 0 & 0\\ 0 & 0 & 0 & 1+v & 0 & 0\\ 0 & 0 & 0 & 0 & 1+v & 0\\ 0 & 0 & 0 & 0 & 0 & 1+v\end{bmatrix}\begin{bmatrix}\sigma_{xx}\\ \sigma_{yy}\\ \sigma_{zz}\\ \sigma_{xy}\\ \sigma_{yz}\\ \sigma_{xz}\end{bmatrix} \qquad \text{Eq. (11.4)}$$

$$\begin{bmatrix}\sigma_{xx}\\ \sigma_{yy}\\ \sigma_{zz}\\ \sigma_{xy}\\ \sigma_{yz}\\ \sigma_{xz}\end{bmatrix}=\frac{E}{(1+v)(1-2v)}\begin{bmatrix}\frac{1-v}{v} & 1 & 1 & 0 & 0 & 0\\ 1 & \frac{1-v}{v} & 1 & 0 & 0 & 0\\ 1 & 1 & \frac{1-v}{v} & 0 & 0 & 0\\ 0 & 0 & 0 & \frac{1-2v}{v} & 0 & 0\\ 0 & 0 & 0 & 0 & \frac{1-2v}{v} & 0\\ 0 & 0 & 0 & 0 & 0 & \frac{1-2v}{v}\end{bmatrix}\begin{bmatrix}\varepsilon_{xx}\\ \varepsilon_{yy}\\ \varepsilon_{zz}\\ \varepsilon_{xy}\\ \varepsilon_{yz}\\ \varepsilon_{xy}\end{bmatrix} \qquad \text{Eq. (11.5)}$$

Finite Element Expression

$$\mathbf{K^e u^e = f_M^e + f_I^e} \qquad \text{Eq. (11.6)}$$

In simple words the sum of the forces **f** (stresses) applied equal the deformation **u** of the object multiplied by a "Stiffness" Matrix **K**.

Derivation of the stiffness matrix: a one D example.

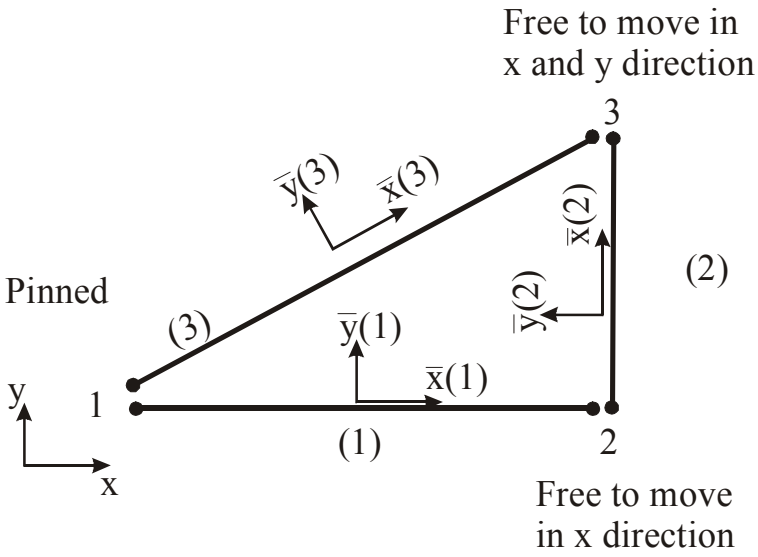


Figure 11-1: Three bars, consider the application of stress in the x direction on node 1, what is the deformation of the entire system?

Local Coordinate System

Later we will discuss the transformation of any shaped element into an element with standard coordinates. At this stage we will consider the transformation of stress in an xy system along bars. The bars have their own local coordinate system. Let us say that the angle between the x direction of the bar and the x direction of the global system is given as θ.

Looking at each node we will have four values to deal with, a force in the x and y direction, and a displacement in the x and y direction. These will be looked at in the local element coordinates then transformed into the global system coordinates. Let $c = \cos\theta$ and $s = \sin\theta$. Then we can write

$$\begin{bmatrix} \bar{u}_{xi} \\ \bar{u}_{yi} \\ \bar{u}_{xj} \\ \bar{u}_{yi} \end{bmatrix} = \begin{bmatrix} c & s & 0 & 0 \\ -s & c & 0 & 0 \\ 0 & 0 & c & s \\ 0 & 0 & -s & c \end{bmatrix} \begin{bmatrix} u_{xi} \\ u_{yi} \\ u_{xj} \\ u_{yi} \end{bmatrix} \qquad \text{Eq. (11.7)}$$

$$\begin{bmatrix} f_{xi} \\ f_{yi} \\ f_{xj} \\ f_{yi} \end{bmatrix} = \begin{bmatrix} c & -s & 0 & 0 \\ s & c & 0 & 0 \\ 0 & 0 & c & -s \\ 0 & 0 & s & c \end{bmatrix} \begin{bmatrix} \bar{f}_{xi} \\ \bar{f}_{yi} \\ \bar{f}_{xj} \\ \bar{f}_{yi} \end{bmatrix} \qquad \text{Eq. (11.8)}$$

Note that in Eq. (11.7) we have element displacement to global displacement, and in Eq. (11.8) we have global forces to element forces.

Let us consider the element level.

$$\overline{f} = \overline{K}\overline{u} \qquad \text{Eq. (11.9)}$$

Applying Hooks laws from Eq. (11.5), for a one dimensional bar being squashed we can write

$$f = K_s d = \frac{EA}{L} d \qquad \text{Eq. (11.10)}$$

where f is the force applied, d is the displacement, A is the cross-sectional area of the bar, L is the length of the bar and K_s is known as the stiffness. The strain is defined as $\frac{du}{dL}$. No expansion in any other dimension is allowed.

We can then write

$$\begin{bmatrix} \overline{f}_{xi} \\ \overline{f}_{yi} \\ \overline{f}_{xj} \\ \overline{f}_{yi} \end{bmatrix} = \frac{EA}{L} \begin{bmatrix} 1 & 0 & -1 & 0 \\ 0 & 0 & 0 & 0 \\ -1 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix} \begin{bmatrix} \overline{u}_{xi} \\ \overline{u}_{yi} \\ \overline{u}_{xj} \\ \overline{u}_{yi} \end{bmatrix} \qquad \text{Eq. (11.11)}$$

$$\overline{\mathbf{K}} = \frac{EA}{L} \begin{bmatrix} 1 & 0 & -1 & 0 \\ 0 & 0 & 0 & 0 \\ -1 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix} \qquad \text{Eq. (11.12)}$$

Now we need to transform local coordinates and movements into global coordinates and movements:-

$$\begin{aligned} f^{(e)} &= \mathbf{K}^{(e)} u^{(e)} \\ u^{(e)} &= \overline{u}^{(e)} \mathbf{T} \\ \overline{f}^{(e)} &= f^{(e)} \mathbf{T}^T \\ \mathbf{K}^{(e)} &= \mathbf{T}^T \overline{\mathbf{K}}^{(e)} \mathbf{T} \end{aligned} \qquad \text{Eq. (11.13)}$$

We can now transform all the element matrices into the global matrix and form the equations to solve them for the unknowns.

Multiplying through we get

$$\mathbf{K}^{(e)} = \frac{E^{(e)} A^{(e)}}{L^{(e)}} \begin{bmatrix} c^2 & sc & -c^2 & -sc \\ sc & s^2 & -sc & -s^2 \\ -c^2 & sc & s^2 & sc \\ -sc & -s^2 & sc & c^2 \end{bmatrix} \qquad \text{Eq. (11.14)}$$

For the system shown in Figure 11-1 we have the following parameters :

Table 2: Parameters for example shown in Figure 11-1

	Element 1		Element 2		Element 3	
	i	j	i	j	i	j
x	0.0	10.0	10.0	10.0	10.0	0.0
y	0.0	0.0	0.0	10.0	10.0	0.0
L	10.0		10.0		14.1	
E	100.0		50.0		282.8	
A	1.0		1.0		1.0	
EA/L	10.0		5.0		20.0	

For the three beams we have the following element matrices:-

$$\begin{bmatrix} \overline{f}_{x1} \\ \overline{f}_{y1} \\ \overline{f}_{x2} \\ \overline{f}_{y2} \end{bmatrix} = 10 \begin{bmatrix} 1 & 0 & -1 & 0 \\ 0 & 0 & 0 & 0 \\ -1 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix} \begin{bmatrix} \overline{u}_{x1} \\ \overline{u}_{y1} \\ \overline{u}_{x2} \\ \overline{u}_{y2} \end{bmatrix} \qquad \text{Eq. (11.15)}$$

$$\begin{bmatrix} \overline{f}_{x2} \\ \overline{f}_{y2} \\ \overline{f}_{x3} \\ \overline{f}_{y3} \end{bmatrix} = 5 \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & -1 \\ 0 & 0 & 0 & 0 \\ 0 & -1 & 0 & 1 \end{bmatrix} \begin{bmatrix} \overline{u}_{x1} \\ \overline{u}_{y1} \\ \overline{u}_{x2} \\ \overline{u}_{y2} \end{bmatrix} \qquad \text{Eq. (11.16)}$$

$$\begin{bmatrix} \overline{f}_{x1} \\ \overline{f}_{y1} \\ \overline{f}_{x3} \\ \overline{f}_{y3} \end{bmatrix} = 20 \begin{bmatrix} \frac{1}{2} & \frac{1}{2} & -\frac{1}{2} & -\frac{1}{2} \\ \frac{1}{2} & \frac{1}{2} & -\frac{1}{2} & -\frac{1}{2} \\ -\frac{1}{2} & -\frac{1}{2} & \frac{1}{2} & \frac{1}{2} \\ -\frac{1}{2} & -\frac{1}{2} & \frac{1}{2} & \frac{1}{2} \end{bmatrix} \begin{bmatrix} \overline{u}_{x1} \\ \overline{u}_{y1} \\ \overline{u}_{x3} \\ \overline{u}_{y3} \end{bmatrix} \qquad \text{Eq. (11.17)}$$

We can now combine the contributions of the individual nodes from each element formulation to arrive at the master stiffness equation:-

$$\begin{bmatrix} f_{x1} \\ f_{y1} \\ f_{x2} \\ f_{y2} \\ f_{x3} \\ f_{y3} \end{bmatrix} = \begin{bmatrix} 20 & 10 & -10 & 0 & -10 & -10 \\ 10 & 10 & 0 & 0 & -10 & -10 \\ -10 & 0 & 10 & 0 & 0 & 0 \\ 0 & 0 & 0 & 5 & 0 & -5 \\ -10 & -10 & 0 & 0 & 10 & 10 \\ 10 & -10 & 0 & -5 & 10 & 15 \end{bmatrix} \begin{bmatrix} u_{x1} \\ u_{y1} \\ u_{x2} \\ u_{y2} \\ u_{x3} \\ u_{y3} \end{bmatrix} \qquad \text{Eq. (11.18)}$$

Let us look at position 1,1 in the stiffness matrix, we have the value 20. This comes from 10 x 1 in Eq. (11.16) plus 20 x ½ in Eq. (11.17). In position 5,5 we have the value 10. This comes from 5 x 0 in Eq. (11.16) + 20 x ½ in Eq. (11.17).

The equation can now be solved as discussed before. Values of *f* and *u* can be set depending on the static conditions.

Stress Recovery.

Just as groundwater velocities needed to be recovered after the equation system had been solved so must the stress be recovered. The stress in an element is a function of the deformation of the element. Once the deformation has been defined so, via Hookes equations Eq. (11.5) can the stress in the individual elements be calculated.

The example above is considered in the spread sheet Example FE Calculations under the sheet "Stress train 1" .

Plane Stress and Plane Strain

If we take a 2D element, then the total strain at any point within the element is defined by the three components which contribute to internal work. Following (Zienkiewicz and Taylor 2000) i.e.

$$\boldsymbol{\varepsilon} = \begin{Bmatrix} \varepsilon_x \\ \varepsilon_y \\ \varepsilon_{xy} \end{Bmatrix} = \begin{bmatrix} \frac{\delta}{\delta x} & 0 \\ 0 & \frac{\delta}{\delta y} \\ \frac{\delta}{\delta x} & \frac{\delta}{\delta y} \end{bmatrix} \begin{Bmatrix} u_x \\ u_y \end{Bmatrix} = \mathbf{Su} \qquad \text{Eq. (11.19)}$$

For a triangular element there are six components of element displacement, two per node in the x and y direction, giving per element the displacement vector **u**. The shape functions can be used to define the displacement at any point

$$\begin{Bmatrix} u_x \\ u_y \end{Bmatrix} = \mathbf{Nu} = \left[\mathbf{I}Ni, \mathbf{I}Nj, \mathbf{I}Nm\right] \qquad \text{Eq. (11.20)}$$

where $I = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$ representing the xy coordinate system

$$\boldsymbol{\varepsilon} = \mathbf{Bu}$$

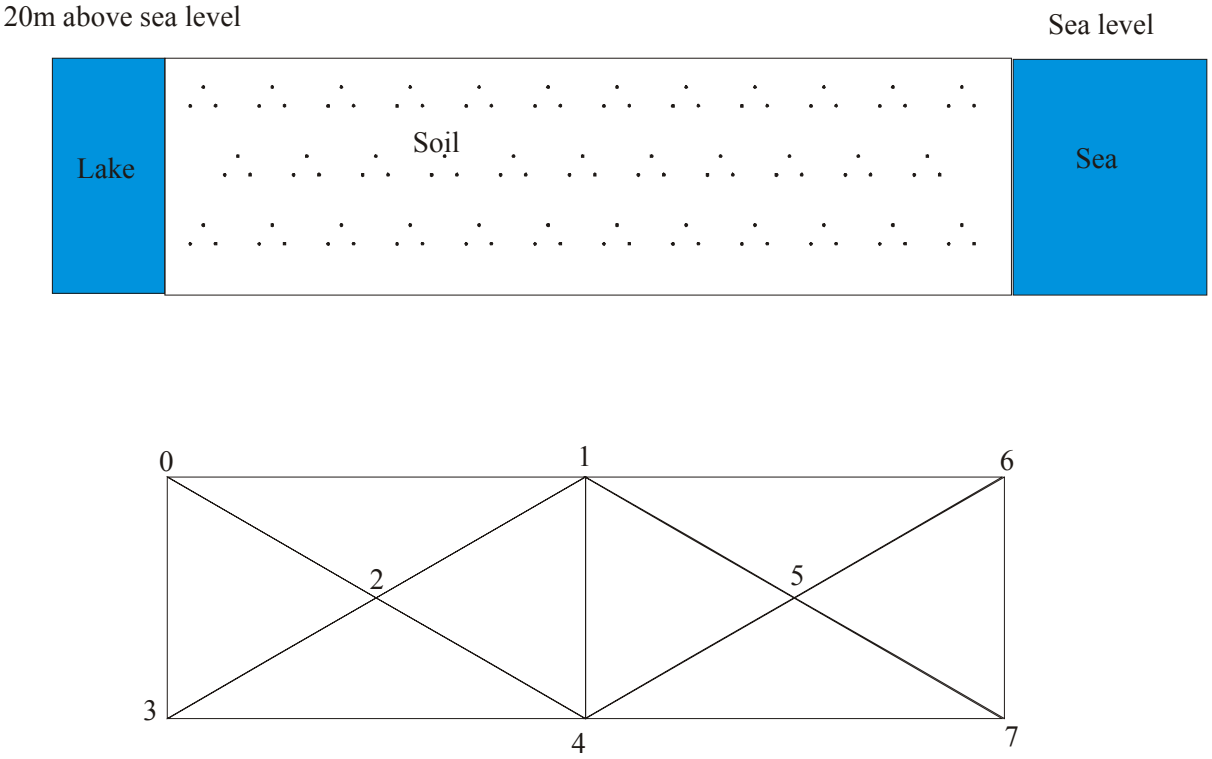
$$\mathbf{B}_i = \mathbf{SN}_i = \begin{bmatrix} \frac{\delta N_i}{\delta x} & 0 \\ 0 & \frac{\delta N_i}{\delta y} \\ \frac{\delta N_i}{\delta x} & \frac{\delta N_i}{\delta y} \end{bmatrix} \qquad \text{Eq. (11.21)}$$

The complete strain matrix for a triangle is then given by

$$\mathbf{B} = \mathbf{SN} = \begin{bmatrix} \frac{\delta N_i}{\delta x} & 0 & \frac{\delta N_j}{\delta x} & 0 & \frac{\delta N_m}{\delta x} & 0 \\ 0 & \frac{\delta N_i}{\delta y} & 0 & \frac{\delta N_j}{\delta y} & 0 & \frac{\delta N_m}{\delta y} \\ \frac{\delta N_i}{\delta x} & \frac{\delta N_i}{\delta y} & \frac{\delta N_j}{\delta x} & \frac{\delta N_j}{\delta y} & \frac{\delta N_m}{\delta x} & \frac{\delta N_m}{\delta y} \end{bmatrix} \qquad \text{Eq. (11.22)}$$

12. Two dimensional stress strain and hydrogeological analysis.

In the introductory section a two dimensional grid comprising triangles was introduced for groundwater flow and for stress strain analysis. Here that grid is taken and applied to provide a hydrogeological and a stress strain model. It should be noted that this is not a poroelastic analysis as the flow and the stress strain terms are not coupled, but it is a introduction to what finite element analysis is capable of. The grid is presented below again for convenience. Both these models are presented in the accompanying excel work sheet.



head at node 0 = 20m
head at node 3 = 20m
head at node 6 = 0m
head at node 7 = 0m

all other heads are not known.

Figure 12-1: Hydrogeological Model

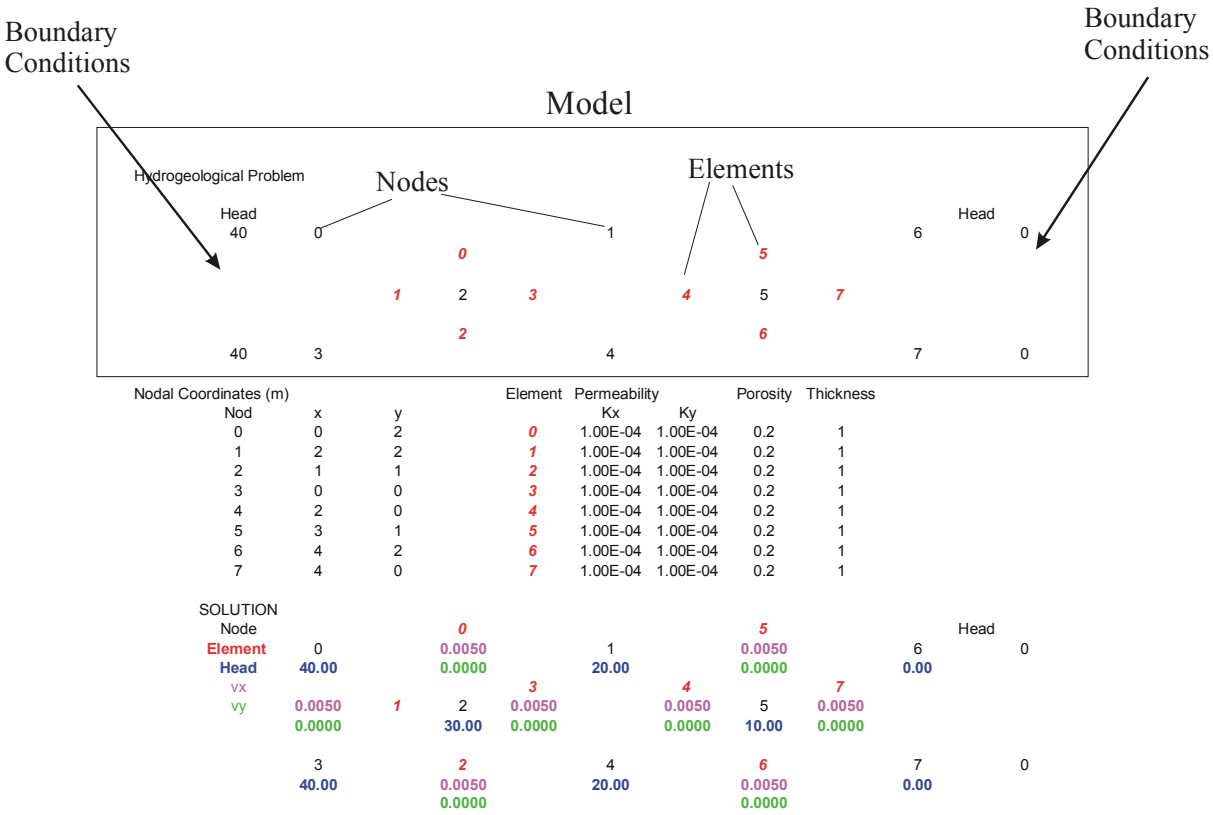


Figure 12-2: Hydrogeological model in excel, cover work sheet.

The hydrogeological model is found under the file "Hydrogeological problem, 2D triangles". The cover worksheet contains the model parameters, details of which element belongs where, what the nodal coordinates are and the solution to the values entered. You can change values in this sheet and see what happens to the solution. Don't forget this application only has 7 elements so don't expect a perfect solution, and take account of the geometry of the system, for instance when trying to trace the flow of ground water in the xy directions. The values are averaged over the elements.

The second work sheet contains the "Global Matrices" Figure 12-3, i.e. combined from the accompanying 7 element work sheets. The individual calculations of all the various parameters and the shape functions have already been discussed. The specific differential and interpolation functions for the triangular element can be found in Kolditz 2001, or Zienkiewicz and Taylor 2000.

K Matrix

	0	1	2	3	4	5	6	7
0	1.00E-04	0.00E+00	-1.00E-04	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
1	0.00E+00	2.00E-04	-1.00E-04	0.00E+00	0.00E+00	-1.00E-04	0.00E+00	0.00E+00
2	-1.00E-04	-1.00E-04	4.00E-04	-1.00E-04	-1.00E-04	0.00E+00	0.00E+00	0.00E+00
3	0.00E+00	0.00E+00	-1.00E-04	1.00E-04	0.00E+00	0.00E+00	0.00E+00	0.00E+00
4	0.00E+00	0.00E+00	-1.00E-04	0.00E+00	2.00E-04	-1.00E-04	0.00E+00	0.00E+00
5	0.00E+00	-1.00E-04	0.00E+00	0.00E+00	-1.00E-04	4.00E-04	-1.00E-04	-1.00E-04
6	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	-1.00E-04	1.00E-04	0.00E+00
7	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	-1.00E-04	0.00E+00	1.00E-04

Boundary Conditions

	heads
0	40
1	
2	
3	40
4	
5	
6	0
7	0

Residue

		Residue
0	0	x
1	0	0.00E+00
2	0	8.00E-03
3	0	x
4	0	0.00E+00
5	0	0.00E+00
6	0	x
7	0	x

Solve for h1,2,4,5

	1	2	3	4
1	2.00E-04	-1.00E-04	0.00E+00	-1.00E-04
2	-1.00E-04	4.00E-04	-1.00E-04	0.00E+00
3	0.00E+00	-1.00E-04	2.00E-04	-1.00E-04
4	-1.00E-04	0.00E+00	-1.00E-04	4.00E-04

h1	0.00E+00
h2	8.00E-03
h4	0.00E+00
h5	0.00E+00

Inverse

7500	2500	2500	2500
2500	3750	2500	1250
2500	2500	7500	2500
2500	1250	2500	3750

Solution

20.00
30.00
20.00
10.00

Total Solution

40	h0
20.00	h1
30.00	h2
40.00	h3
20.00	h4
10.00	h5
0	h6
0	h7

Check Inverse

1.00E+00	0.00E+00	0.00E+00	0.00E+00
1.11E-16	1.00E+00	1.11E-16	0.00E+00
0.00E+00	0.00E+00	1.00E+00	0.00E+00
0.00E+00	0.00E+00	0.00E+00	1.00E+00

Recover Velocities

Element	Direction	Darcy Velocities	Advective Velocities
0	x	1.00E-03	5.00E-03
0	y	0.00E+00	0.00E+00
1	x	1.00E-03	5.00E-03
1	y	0.00E+00	0.00E+00
2	x	1.00E-03	5.00E-03
2	y	0.00E+00	0.00E+00
3	x	1.00E-03	5.00E-03
3	y	0.00E+00	0.00E+00
4	x	1.00E-03	5.00E-03
4	y	0.00E+00	0.00E+00
5	x	1.00E-03	5.00E-03
5	y	1.78E-19	8.88E-19
6	x	1.00E-03	5.00E-03
6	y	0.00E+00	0.00E+00
7	x	1.00E-03	5.00E-03
7	y	0.00E+00	0.00E+00

Figure 12-3: Global matrices from hydrogeological example.

Element 0

Nod	x	y		
0	0	2		i
2	1	1		j
1	2	2		m

Shape Function

ai	0		aj	4		am	-2	
bi	-1		bj	0		bm	1	
ci	1		cj	-2		cm	1	

Area

							dx	dy
1	0	2				dNi	-0.5	0.5
1	1	1		Area	1	dNj	0	-1
1	2	2				dNm	0.5	0.5

Porosity	0.2	Thickness	1
Kx	1.00E-04		
Ky	1.00E-04		

-0.5	0.5	
0	-1	
0.5	0.5	

1.00E-04	0
0	1.00E-04

-0.5	0	0.5
0.5	-1	0.5

-5.00E-05	5.00E-05	
0.00E+00	-1.00E-04	
5.00E-05	5.00E-05	

5.00E-05	-5.00E-05	0.00E+00
-5.00E-05	1.00E-04	-5.00E-05
0.00E+00	-5.00E-05	5.00E-05

K(e)

	0	**2**	**1**
0	5.00E-05	-5.00E-05	0.00E+00
2	-5.00E-05	1.00E-04	-5.00E-05
1	0.00E+00	-5.00E-05	5.00E-05

	0	**1**	**2**	**3**	**4**	**5**	**6**	**7**
0	5.00E-05	0.00E+00	-5.00E-05					
1	0.00E+00	5.00E-05	-5.00E-05					
2	-5.00E-05	-5.00E-05	1.00E-04					
3								
4								
5								
6								
7								

Recover Velocities

Element		
0	x	1.00E-03
0	y	0.00E+00
1	x	
1	y	
2	x	
2	y	
3	x	
3	y	
4	x	
4	y	
5	x	
5	y	
6	x	
6	y	
7	x	
7	y	

Solved Heads

h0	40
h1	20
h2	30
h3	40
h4	20
h5	10
h6	0
h7	0

Velocity Calculations

	dx	dy	**Nodes**
dNi	-0.5	0.5	0
dNj	0	-1	2
dNm	0.5	0.5	1

Element 0

dh/dx	-10
dy/dx	0

Figure 12-4: Element matrix for hydrogeological example.

Stress strain analysis

The conceptual model is presented in Figure 12-5

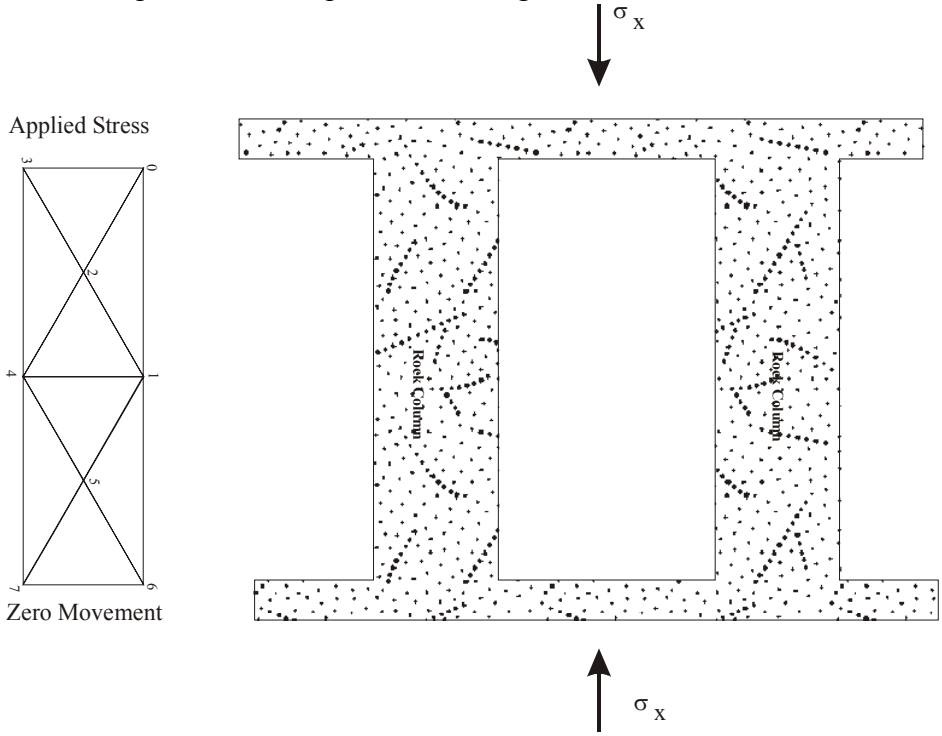
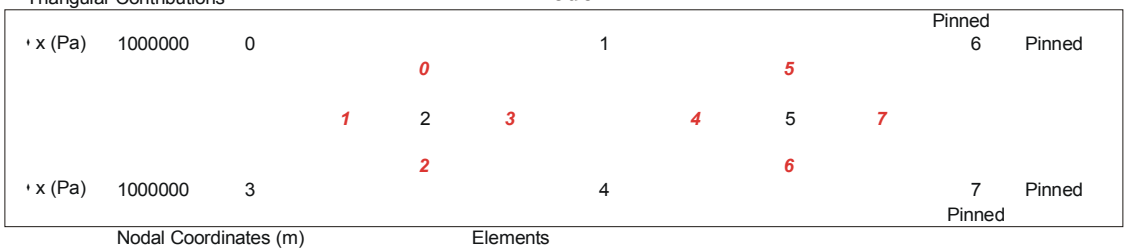


Figure 12-5: Analysis of deformation of column under applied stress.

The excel sheet "Stress Strain Problem 2D Triangles" comprises again a cover sheet with the model details, a global matrices sheet Figure 12-6, and then the individual element matrices Figure 12-7.

Stress Strain Problems
Triangular Contributions

Model



Nodal Coordinates (m)

Node	x	y
0	0	2
1	2	2
2	1	1
3	0	0
4	2	0
5	3	1
6	4	2
7	4	0

Elements

Element	Nodes
0	0 2 1
1	3 2 0
2	3 4 2
3	2 4 1
4	4 5 1
5	1 5 6
6	4 7 5
7	5 7 6

For element parameters see actual element (E, v, thickness)

Solution

Displacements (m)

0x	0.00395588
0y	0.00023529
1x	0.00194853
1y	0.00029412
2x	0.00295956
2y	3.8844E-10
3x	0.00395588
3y	-0.0002353
4x	0.00194853
4y	-0.0002941
5x	0.0009375
5y	2.0244E-10
6x	0
6y	0
7x	0
7y	0

Stress (Pa)

Element	0	1	2	3	4	5	6	7
' x	-1.00E+06	-1.00E+06	-1.00E+06	-1.00E+06	-1.00E+06	-1.00E+06	-1.00E+06	-1.00E+06
' y	1.47E+04	-1.47E+04	1.47E+04	4.41E+04	4.41E+04	-1.03E+05	-1.03E+05	-2.50E+05
xy	8.27E-06	-8.84E-11	-8.27E-06	6.79E-11	-1.38E-10	-4.14E-05	4.14E-05	-7.59E-11

Figure 12-6: Stress strain model in excel, cover page.

Again it is possible to change the various parameters to see what happens in the model. The shape functions and the derivatives are identical to the hydrogeological functions. The mathematics and construction of the global matrices is slightly different and the work sheets slightly more complicated, but in principal the method is identical.

K Matrix

		1	2	3	4	5	6	7	8	9	10	11	12
		0x	0y	1x	1y	2x	2y	3x	3y	4x	4y	5x	5y
1	0x	533333334	-133333334	-266666667	-66666667	-533333334	133333334	266666667	66666666.6	0	0	0	0
2	0y	-133333334	533333334	66666666.6	266666667	133333334	-533333334	-66666667	-266666667	0	0	0	0
3	1x	-266666667	66666666.6	1066666667	0	-533333334	-133333334	0	0	533333333	0	-533333334	133333334
4	1y	-66666667	266666667	0	1066666667	-133333334	-533333334	0	0	0	-533333333	133333334	-533333334
5	2x	-533333334	133333334	-533333334	-133333334	2133333334	0	-533333334	-133333334	-533333334	133333334	0	0
6	2y	133333334	-533333334	-133333334	-533333334	0	2133333334	-133333334	-533333334	133333334	-533333334	0	0
7	3x	266666667	-66666667	0	0	-533333334	-133333334	533333334	133333334	-266666667	66666666.6	0	0
8	3y	66666666.6	-266666667	0	0	-133333334	-533333334	133333334	533333334	-66666667	266666667	0	0
9	4x	0	0	533333333	0	-533333334	133333334	-266666667	-66666667	1066666667	0	-533333334	-133333334
10	4y	0	0	0	-533333333	133333334	-533333334	66666666.6	266666667	0	1066666667	-133333334	-533333334
11	5x	0	0	-533333334	133333334	0	0	0	0	-533333334	-133333334	2133333334	0
12	5y	0	0	133333334	-533333334	0	0	0	0	-133333334	-533333334	0	2133333334
13	6x	0	0	-266666667	66666666.6	0	0	0	0	0	0	-533333334	-133333334
14	6y	0	0	-66666667	266666667	0	0	0	0	0	0	-133333334	-533333334
15	7x	0	0	0	0	0	0	0	0	-266666667	-66666667	-533333334	133333334
16	7y	0	0	0	0	0	0	0	0	66666666.6	266666667	133333334	-533333334

Boundary Conditions Forces

0x	20
0y	0
1x	0
1y	0
2x	0
2y	0
3x	20
3y	0
4x	0
4y	0
5x	0
5y	0
6x	?
6y	?
7x	?
7y	?

Boundary Conditions Movement

0x	?
0y	?
1x	?
1y	?
2x	?
2y	?
3x	?
3y	?
4x	?
4y	?
5x	?
5y	?
6x	0
6y	0
7x	0
7y	0

Solve for unknown displacments

	0 0x	0y	1x	1y	2x	2y	3x	3y	4x	4y	5x
0x	533333334	-133333334	-266666667	-66666667	-533333334	133333334	266666667	66666666.6	0	0	0
0y	-133333334	533333334	66666666.6	266666667	133333334	-533333334	-66666667	-266666667	0	0	0
1x	-266666667	66666666.6	1066666667	0	-533333334	-133333334	0	0	533333333	0	-533333334
1y	-66666667	266666667	0	1066666667	-133333334	-533333334	0	0	0	-533333333	133333334
2x	-533333334	133333334	-533333334	-133333334	2133333334	0	-533333334	-133333334	-533333334	133333334	0
2y	133333334	-533333334	-133333334	-533333334	0	2133333334	-133333334	-533333334	133333334	-533333334	0
3x	266666667	-66666667	0	0	-533333334	-133333334	533333334	133333334	-266666667	66666666.6	0
3y	66666666.6	-266666667	0	0	-133333334	-533333334	133333334	533333334	-66666667	266666667	0
4x	0	0	533333333	0	-533333334	133333334	-266666667	-66666667	1066666667	0	-533333334
4y	0	0	0	-533333333	133333334	-533333334	66666666.6	266666667	0	1066666667	-133333334
5x	0	0	-533333334	133333334	0	0	0	0	-533333334	-133333334	2133333334
5y	0	0	133333334	-533333334	0	0	0	0	-133333334	-533333334	0

Inverse

	1	2	3	4	5	6	7	8	9	10	11
1	5.9779E-09	8.1176E-09	2.9743E-09	2.1471E-09	1.4798E-09	4.75E-09	-2.022E-09	7.8824E-09	-1.026E-09	1.8529E-09	4.6875E-10
2	8.1176E-09	5.33333261	5.9706E-09	2.66666582	-5.882E-11	3.99999922	-7.882E-09	5.33333261	-6.029E-09	2.66666582	1.3601E-16
3	2.9743E-09	5.9706E-09	2.9596E-09	2.0882E-09	9.8162E-10	4E-09	-1.026E-09	6.0294E-09	-1.04E-09	1.9118E-09	4.6875E-10
4	2.1471E-09	2.66666596	2.0882E-09	2.66666566	1.7647E-10	2.66666581	-1.853E-09	2.66666596	-1.912E-09	2.66666566	9.1807E-17
5	1.4798E-09	-5.882E-11	9.8162E-10	1.7647E-10	1.7289E-09	1.5848E-16	1.4798E-09	5.8824E-11	9.8162E-10	-1.765E-10	4.6875E-10
6	4.75E-09	3.99999915	4E-09	2.66666574	2.778E-16	3.33333245	-4.75E-09	3.99999915	-4E-09	2.66666574	1.1392E-16
7	-2.022E-09	-7.882E-09	-1.026E-09	-1.853E-09	1.4798E-09	-4.75E-09	5.9779E-09	-8.118E-09	2.9743E-09	-2.147E-09	4.6875E-10
8	7.8824E-09	5.33333229	6.0294E-09	2.66666582	5.8824E-11	3.99999906	-8.118E-09	5.33333229	-5.971E-09	2.66666582	1.3598E-16
9	-1.026E-09	-6.029E-09	-1.04E-09	-1.912E-09	9.8162E-10	-4E-09	2.9743E-09	-5.971E-09	2.9596E-09	-2.088E-09	4.6875E-10
10	1.8529E-09	2.66666533	1.9118E-09	2.66666566	-1.765E-10	2.66666549	-2.147E-09	2.66666533	-2.088E-09	2.66666566	9.19E-17
11	4.6875E-10	-2.903E-17	4.6875E-10	3.0475E-17	4.6875E-10	7.3609E-19	4.6875E-10	-2.907E-17	4.6875E-10	3.0568E-17	7.0312E-10
12	7.5E-10	1.33333295	7.5E-10	1.33333283	1.0852E-16	1.33333289	-7.5E-10	1.33333295	-7.5E-10	1.33333283	4.5927E-17

Check Inverse

0.99999989	-38.9534	-7.45E-08	-2.384E-07	-5.802E-09	-19.4767	7.9361E-08	-38.9534	4.8659E-08	-1.788E-07	-6.556E-17
4.3093E-07	156.813601	2.9802E-07	7.1526E-07	2.3207E-08	77.9068007	-3.174E-07	155.813601	-1.946E-07	4.7684E-07	8.8751E-18
5.1684E-08	14.2422345	1.00000004	0	1.0357E-10	7.12111729	-3.499E-08	14.2422344	-2.397E-08	0	7.3328E-18
1.1003E-06	423.321941	6.7357E-07	1.00000048	4.6544E-08	211.66097	-9.228E-07	423.321941	-5.838E-07	0	-1.738E-17
-1.113E-07	-42.165919	-6.198E-08	2.9802E-07	1	-21.082959	1.0696E-07	-42.165919	7.2589E-08	2.9802E-07	2.791E-16
1.2183E-07	226.589479	1.5327E-07	-1.669E-06	6.945E-09	114.294739	-5.665E-07	226.58948	-3.893E-07	-9.537E-07	1.0807E-17
-1.23E-07	-67.277085	-9.366E-08	-5.96E-08	-6.67E-09	-33.638543	1.00000015	-67.277086	9.7315E-08	-5.96E-08	-8.585E-17
-4.918E-07	-269.10834	-3.747E-07	4.7684E-07	-2.668E-08	-134.55417	6.0069E-07	-268.10834	3.8926E-07	4.7684E-07	-5.288E-18
-7.921E-09	7.04464659	-8.302E-09	0	2.9973E-09	3.52232325	-9.023E-09	7.04464662	1	0	-6.284E-17
-1.461E-06	-678.70177	-1.03E-06	0	-4.191E-08	-339.35089	1.5931E-06	-678.70177	1.0551E-06	1.00000012	1.038E-17
1.9882E-07	84.7396824	1.3057E-07	5.4091E-09	6.3379E-09	42.3698412	-1.95E-07	84.7396825	-1.274E-07	5.6076E-09	1
5.9867E-07	284.170182	5.6046E-07	0	-1.621E-08	142.085091	-7.742E-07	284.170183	-5.534E-07	0	1.7858E-17

Solve for U

5.9779E-09	8.1176E-09	2.9743E-09	2.1471E-09	1.4798E-09	4.75E-09	-2.022E-09	7.8824E-09	-1.026E-09	1.8529E-09	4.6875E-10
8.1176E-09	5.33333261	5.9706E-09	2.66666582	-5.882E-11	3.99999922	-7.882E-09	5.33333261	-6.029E-09	2.66666582	1.3601E-16
2.9743E-09	5.9706E-09	2.9596E-09	2.0882E-09	9.8162E-10	4E-09	-1.026E-09	6.0294E-09	-1.04E-09	1.9118E-09	4.6875E-10
2.1471E-09	2.66666596	2.0882E-09	2.66666566	1.7647E-10	2.66666581	-1.853E-09	2.66666596	-1.912E-09	2.66666566	9.1807E-17
1.4798E-09	-5.882E-11	9.8162E-10	1.7647E-10	1.7289E-09	1.5848E-16	1.4798E-09	5.8824E-11	9.8162E-10	-1.765E-10	4.6875E-10
4.75E-09	3.99999915	4E-09	2.66666574	2.778E-16	3.33333245	-4.75E-09	3.99999915	-4E-09	2.66666574	1.1392E-16
-2.022E-09	-7.882E-09	-1.026E-09	-1.853E-09	1.4798E-09	-4.75E-09	5.9779E-09	-8.118E-09	2.9743E-09	-2.147E-09	4.6875E-10
7.8824E-09	5.33333229	6.0294E-09	2.66666582	5.8824E-11	3.99999906	-8.118E-09	5.33333229	-5.971E-09	2.66666582	1.3598E-16
-1.026E-09	-6.029E-09	-1.04E-09	-1.912E-09	9.8162E-10	-4E-09	2.9743E-09	-5.971E-09	2.9596E-09	-2.088E-09	4.6875E-10
1.8529E-09	2.66666533	1.9118E-09	2.66666566	-1.765E-10	2.66666549	-2.147E-09	2.66666533	-2.088E-09	2.66666566	9.19E-17
4.6875E-10	-2.903E-17	4.6875E-10	3.0475E-17	4.6875E-10	7.3609E-19	4.6875E-10	-2.907E-17	4.6875E-10	3.0568E-17	7.0312E-10
7.5E-10	1.33333295	7.5E-10	1.33333283	1.0852E-16	1.33333289	-7.5E-10	1.33333295	-7.5E-10	1.33333283	4.5927E-17

Solve for unknown forces

	0x	0y	1x	1y	2x	2y	3x	3y	4x	4y	5x	5y
0x	533333334	-133333334	-266666667	-66666667	-533333334	133333334	266666667	66666666.6	0	0	0	0
0y	-133333334	533333334	66666666.6	266666667	133333334	-533333334	-66666667	-266666667	0	0	0	0
1x	-266666667	66666666.6	1066666667	0	-533333334	-133333334	0	0	533333333	0	-533333334	133333334
1y	-66666667	266666667	0	1066666667	-133333334	-533333334	0	0	0	-533333333	133333334	-533333334
2x	-533333334	133333334	-533333334	-133333334	2133333334	0	-533333334	-133333334	-533333334	133333334	0	0
2y	133333334	-533333334	-133333334	-533333334	0	2133333334	-133333334	-533333334	133333334	-533333334	0	0
3x	266666667	-66666667	0	0	-533333334	-133333334	533333334	133333334	-266666667	66666666.6	0	0
3y	66666666.6	-266666667	0	0	-133333334	-533333334	133333334	533333334	-66666667	266666667	0	0
4x	0	0	533333333	0	-533333334	133333334	-266666667	-66666667	1066666667	0	-533333334	-133333334
4y	0	0	0	-533333333	133333334	-533333334	66666666.6	266666667	0	1066666667	-133333334	-533333334
5x	0	0	-533333334	133333334	0	0	0	0	-533333334	-133333334	2133333334	0
5y	0	0	133333334	-533333334	0	0	0	0	-133333334	-533333334	0	2133333334
6x	0	0	-266666667	66666666.6	0	0	0	0	0	0	-533333334	-133333334
6y	0	0	-66666667	266666667	0	0	0	0	0	0	-133333334	-533333334
7x	0	0	0	0	0	0	0	0	-266666667	-66666667	-533333334	133333334
7y	0	0	0	0	0	0	0	0	66666666.6	266666667	133333334	-533333334

Recovering Stresses

Element	0	1	2	3	4	5	6	7
' x	-1.00E+06	-1.00E+06	-1.00E+06	-1.00E+06	-1.00E+06	-1.00E+06	-1.00E+06	-1.00E+06
' y	1.47E+04	-1.47E+04	1.47E+04	4.41E+04	4.41E+04	-1.03E+05	-1.03E+05	-2.5E+05
xy	8.27E-06	-8.84E-11	-8.27E-06	6.79E-11	-1.38E-10	-4.14E-05	4.14E-05	-7.59E-11

Figure 12-7: Global matrices sheet of stress strain analysis.

Element 0

Nod	x	y	
0	0	2	i
2	1	1	j
1	2	2	m

Shape Function

ai	0	aj	4	am	-2		
bi	-1	bj	0	bm	1		
ci	1	cj	-2	cm	1		

Area

						dx	dy
1	0	2			dNi	-0.5	0.5
1	1	1	Area	1	dNj	0	-1
1	2	2			dNm	0.5	0.5

Strain Matrix B=SN Correct

-0.5	0	0	0	0.5	0
0	0.5	0	-1	0	0.5
0.5	-0.5	-1	0	0.5	0.5

Elasticity Matrix (Plane Stress) D Correct

v=	0.25
E=	1.0E+09
E/(1-v²)	1066666667

1066666667	266666667	0
266666667	1066666667	0
0	0	0.375

Thickness h 1

K

BT

-0.5	0	0.5
0	0.5	-0.5
0	0	-1
0	-1	0
0.5	0	0.5
0	0.5	0.5

0.25

D

1066666667	266666667	0
266666667	1066666667	0
0	0	0.375

B

-0.5	0	0	0	0.5	0
0	0.5	0	-1	0	0.5
0.5	-0.5	-1	0	0.5	0.5

BT D

-533333333	-133333333	0.1875
133333333	533333333	-0.1875
0	0	-0.375
-266666667	-1.067E+09	0
533333333	133333333	0.1875
133333333	533333333	0.1875

BTD B

266666667	-66666667	-0.1875	133333333	-266666667	-66666667
-66666667	266666667	0.1875	-533333333	66666666.6	266666667
-0.1875	0.1875	0.375	0	-0.1875	-0.1875
133333333	-533333333	0	1066666667	-133333333	-533333333
-266666667	66666666.6	-0.1875	-133333333	266666667	66666666.8
-66666667	266666667	-0.1875	-533333333	66666666.8	266666667

	0	0	2	2	1	1	
	266666667	-66666667	-0.1875	133333333	-266666667	-66666667	0
	-66666667	266666667	0.1875	-533333333	66666666.6	266666667	0
1	-0.1875	0.1875	0.375	0	-0.1875	-0.1875	2
	133333333	-533333333	0	1066666667	-133333333	-533333333	2
	-266666667	66666666.6	-0.1875	-133333333	266666667	66666666.8	1
	-66666667	266666667	-0.1875	-533333333	66666666.8	266666667	1

F(e)

	b		**f(e)**
0.33333333	1	=	0.33333333
	1		0.33333333
	1		0.33333333
	1		0.33333333
	1		0.33333333
	1		0.33333333

		1	2	3	4	5	6	7	8	9	10	11	12
		0x	0y	1x	1y	2x	2y	3x	3y	4x	4y	5x	5y
1	0x	266666667	-66666667	-266666667	-66666667	-0.1875	133333333						
2	0y	-66666667	266666667	66666666.6	266666667	0.1875	-533333333						
3	1x	-266666667	66666666.6	266666667	66666666.8	-0.1875	-133333333						
4	1y	-66666667	266666667	66666666.8	266666667	-0.1875	-533333333						
5	2x	-0.1875	0.1875	-0.1875	-0.1875	0.375	0						
6	2y	133333333	-533333333	-133333333	-533333333	0	1066666667						
7	3x												
8	3y												
9	4x												
10	4y												
11	5x												
12	5y												
13	6x												
14	6y												
15	7x												
16	7y												

Stress Recovery

Nod	Disp	
0	3.96E-03	x
0	2.35E-04	y
2	2.96E-03	x
2	3.88E-10	y
1	1.95E-03	x
1	2.94E-04	y

B

-0.5	0	0	0	0.5	0
0	0.5	0	-1	0	0.5
0.5	-0.5	-1	0	0.5	0.5

Ba

-1.00E-03
2.65E-04
2.21E-05

D

1066666667	266666667	0
266666667	1066666667	0
0	0	0.375

Figure 12-8: Element matrices for stress strain example.

13. Jacobian Transformation and Gauss Quadrature

Who`s Jacobi?

Anybody who thought to date that Jacobian was actually a rather nice type of coffee, is about to get a supprise. You will need quite a bit of coffee to get to grips with this so you can use Jacobian matrices without having the feeling in your stomach that you are not really sure what is going on, but it is worth it. Coupled with the Gauss quadrature these techniques form a fundermental part of todays finite element analysis.

Putting the procedure in simple terms a coordinate transformation is applied to convert our element, which can be any shape or form into a regular standard element with coordinates from –1 to +1, and then the Gauss Quadrature is used to find the integral of some function across this standard or „Isoparemetric“ element. The Jacobian for this parametric transformation is calculated and then is reused to transfer this integral back into the real coordinates and make the value usable in the global matrix calculations.

In other words the interpolation functions and their derivates are defined in local coordinates system while the integral formulations for the element matrices are defined in a global coordinate system.

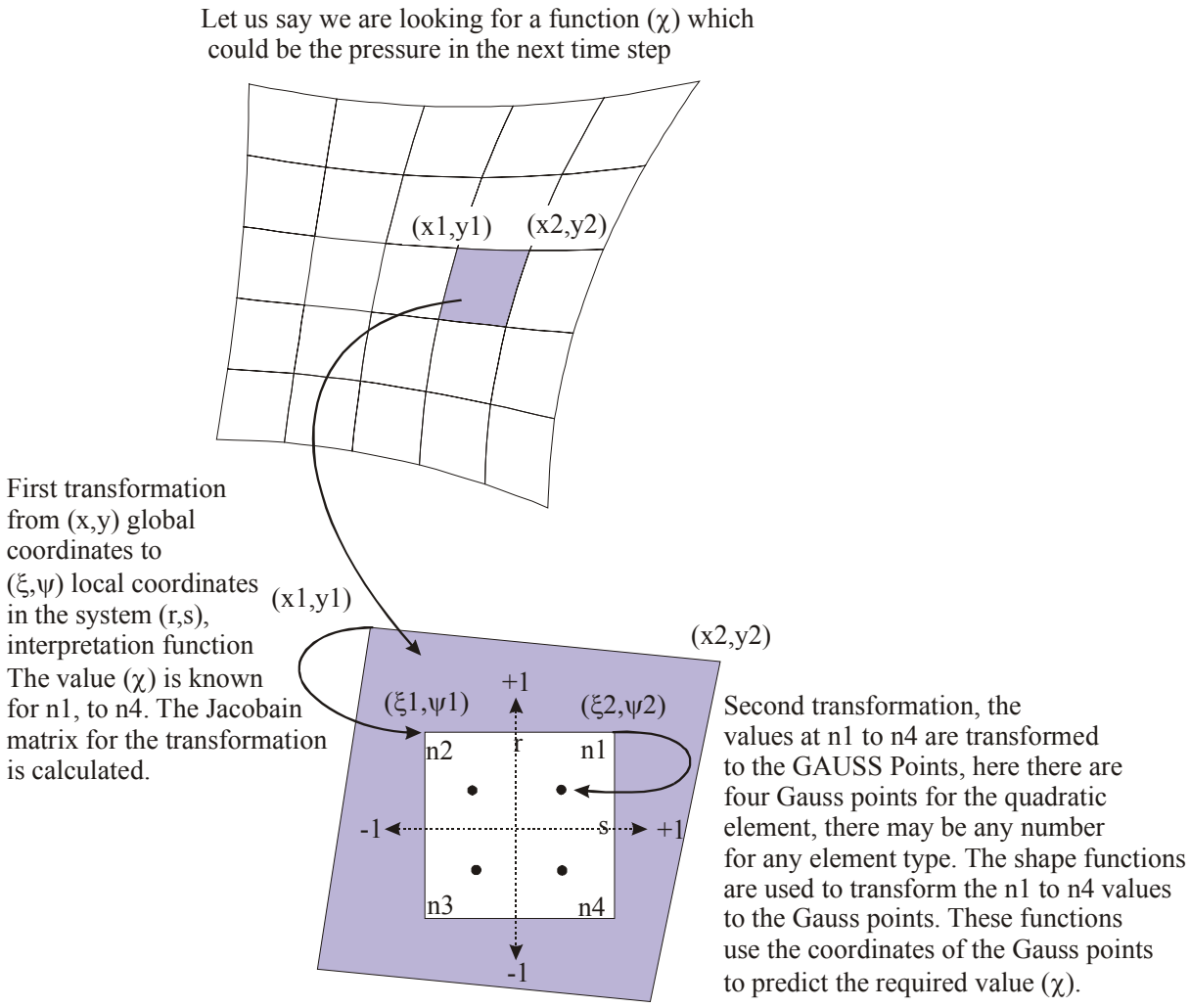
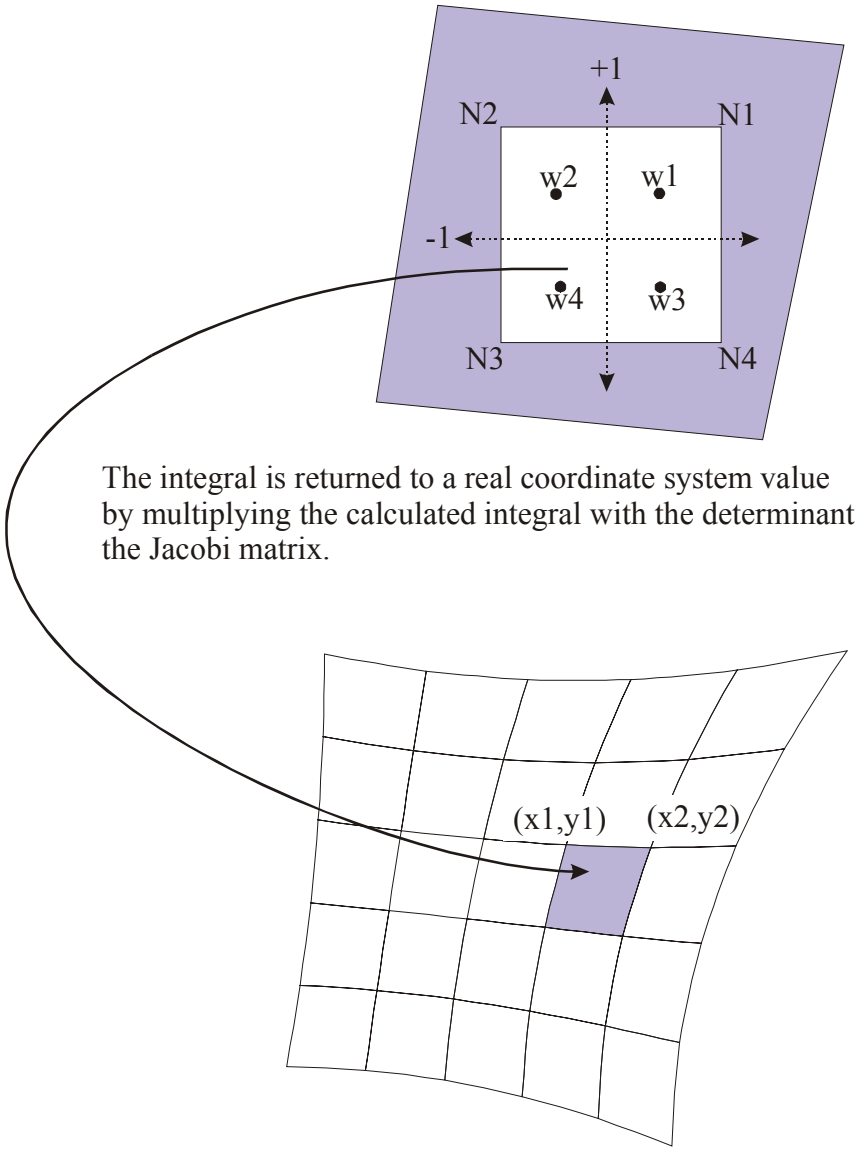


Figure 13-1: From real coordinates to “Isoparemetric” coordinates.

The location of the Gauss points is a constant value depending on the number of gauss points. Each Gauss point receives a weighting w depending on its location. The integral is then the weighted sum of the field value required.



The integral is returned to a real coordinate system value by multiplying the calculated integral with the determinant of the Jacobi matrix.

Figure 13-2: From the Isoparemetric element back to real coordinate system values.

The Jacobian matrix in action:

Let us transfer polar coordinates to Cartesian coordinates.

$$dx = \frac{\delta x}{\delta r} dr + \frac{\delta x}{\delta \theta} d\theta$$
$$dy = \frac{\delta y}{\delta r} dr + \frac{\delta y}{\delta \theta} d\theta \qquad \text{Eq. (13.1)}$$

$$\begin{pmatrix} dx \\ dy \end{pmatrix} = \begin{pmatrix} \frac{\delta x}{\delta r} & \frac{\delta x}{\delta \theta} \\ \frac{\delta y}{\delta r} & \frac{\delta y}{\delta \theta} \end{pmatrix} \begin{pmatrix} dr \\ d\theta \end{pmatrix} \qquad \text{Eq. (13.2)}$$

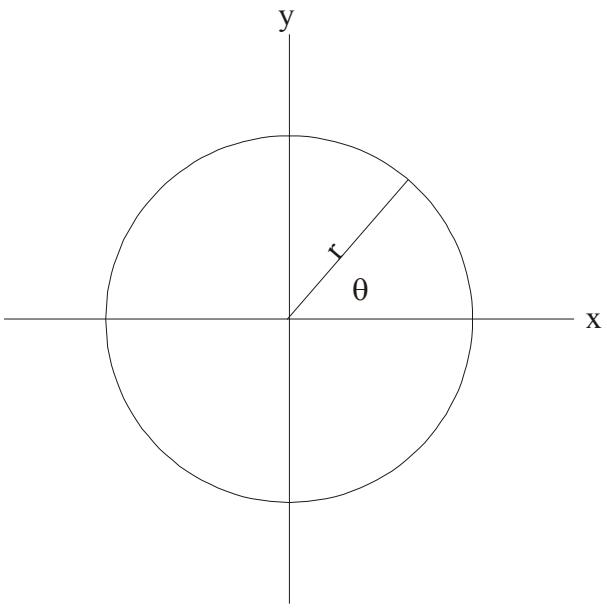


Figure 13-3: Polar and Cartesian coordinates.

$$\begin{aligned} \frac{\delta x}{\delta r} &= \cos\theta \\ \frac{\delta y}{\delta r} &= \sin\theta \\ \frac{\delta x}{\delta \theta} &= -r\sin\theta \\ \frac{\delta y}{\delta \theta} &= r\cos\theta \end{aligned} \qquad \text{Eq. (13.3)}$$

This means we can write the Jacobian as

$$\begin{pmatrix} \cos\theta & -r\sin\theta \\ \sin\theta & r\cos\theta \end{pmatrix} \qquad \text{Eq. (13.4)}$$

Integrating in drdθ and transferring to original dxdy coordinates is then possible

$$dxdy = \left|\det J\right| drd\theta \qquad \text{Eq. (13.5)}$$

So in this case det J is $r\cos(\theta)^2 \; + \; r \; \sin(\theta)^2$

Let us take the one D example. We real coordinates x_1 and x_2. They map to coordinates r_1 =-1 and r_2=+1.

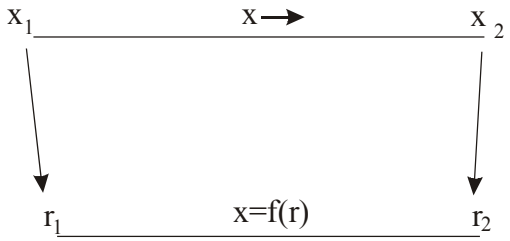


Figure 13-4: Transferring from real xy coordinates to local rs coordinates.

x is a function of r in the rs coordinate system, therefore we write

$$x(r) = a_1 + a_2 r \qquad \text{Eq. (13.6)}$$

Therefore by definition

$$\begin{aligned} x_1 &= a_1 + a_2 r_1 \\ x_2 &= a_1 + a_2 r_2 \end{aligned} \qquad \text{Eq. (13.7)}$$

The Jacobian is then $\frac{dx}{dr} = a_2$

Solving Eq. (13.7) for a_2 gives us

$$a_2 = \frac{x_2 - x_1}{2} = \frac{L}{2} \qquad \text{Eq. (13.8)}$$

in a 1D system det J=J.

A simple example would be storage, let us say we want to know how much water will go into storage for a head change of 2m on both sides of the element. Let us say x_1 is positioned at 50m and x_2 at 75m. The storage we will set at 0.1m. Working in natural coordinates we see that the water going into storage will be 0.1 x 2 x 25=5m³ assuming a 1m depth and height. Now applying the Jacobie transformation:- we move from –1 to +1m, and have a 2m head change, therefore in local co-ordinates 0.1 x 2 x 2=0.4m³ will go into storage. Now this value is converted back to the real co-ordinate system by multiplying by the determinant:- 0.4 x 25/2=5m³.

Repeating this now for a 2D square element aligned with the real coordinate system.

$$\begin{aligned} x(r) &= a_1 + a_2 r \\ y(s) &= b_1 + b_2 r \end{aligned} \qquad \text{Eq. (13.9)}$$

The Jacobian is then

$$\begin{pmatrix} \frac{\delta x}{\delta r} & \frac{\delta x}{\delta s} \\ \frac{\delta y}{\delta r} & \frac{\delta y}{\delta s} \end{pmatrix} = \begin{pmatrix} a_2 & 0 \\ 0 & b_2 \end{pmatrix} \qquad \text{Eq. (13.10)}$$

Solving for a_2 and b_2 gives us

$$a_2 = \frac{x_2 - x_1}{2}$$
$$b_2 = \frac{y_2 - y_1}{2}$$

Eq. (13.11)

detJ=$a_2 b_2$. The example given above can be repeated. Should the system be rotated or deformed then there will be a non diagonal contribution to the Jacobian matrix.

Where the elements become deformed and the coordinate systems are no longer directly lined up it is necessary to resort to given proven formulas for calculating the Jacobian matrices, many of which are given by Istok 1989

The value of the Jacobian varies from point to point within the element because the interpolation function derivatives are themselves functions of the local coordinate system.

14. Gauss Quadrature Example

Gauss quadrature belongs to the methods of numerically integrating functions. In this method a numerical approximation of the integral is obtained by calculating the value of the function at a number of predefined points, weighted sum of these values gives the integral value.

In three dimensions this can be written as

$$\int_{-1}^{1}\int_{-1}^{1}\int_{-1}^{1} f(rst)drdsdt = \sum_{i=1}^{n_r}\sum_{j=1}^{n_s}\sum_{k=1}^{n_t} w_i(r_i)w_j(r_j)w_k(r_k)f(r_i s_j t_k) \qquad \text{Eq. (14.1)}$$

In Eq. (14.1) n is the number of Gauss points. The number and associated position and weighting of these points are given in standard tables. As a rule the number of gauss points necessary to calculate the integral is (n+1)/2, where here n refers to the order of the interpretation polynomial.
Combined use of Gaussian quadrature and Jacobian.

The first step is to determine the highest order polynomial.

The interpolation function is $N_i = \frac{1}{4}(1 + r_i r)(1 + s_i s)$. We find in the matrix calculations that we have NiNi as a function, therefore we have a square of the values r or s. The highest order is therefore 2, which means we need 1.5....2 Guass points.

The coordiantes of these Gauss points are

$$\begin{matrix} -\frac{1}{\sqrt{3}} & -\frac{1}{\sqrt{3}} \\ -\frac{1}{\sqrt{3}} & +\frac{1}{\sqrt{3}} \\ +\frac{1}{\sqrt{3}} & +\frac{1}{\sqrt{3}} \\ +\frac{1}{\sqrt{3}} & -\frac{1}{\sqrt{3}} \end{matrix}$$

Now we need to calculate the Jacobian: We take an example of a warped 2D quadratic element:-

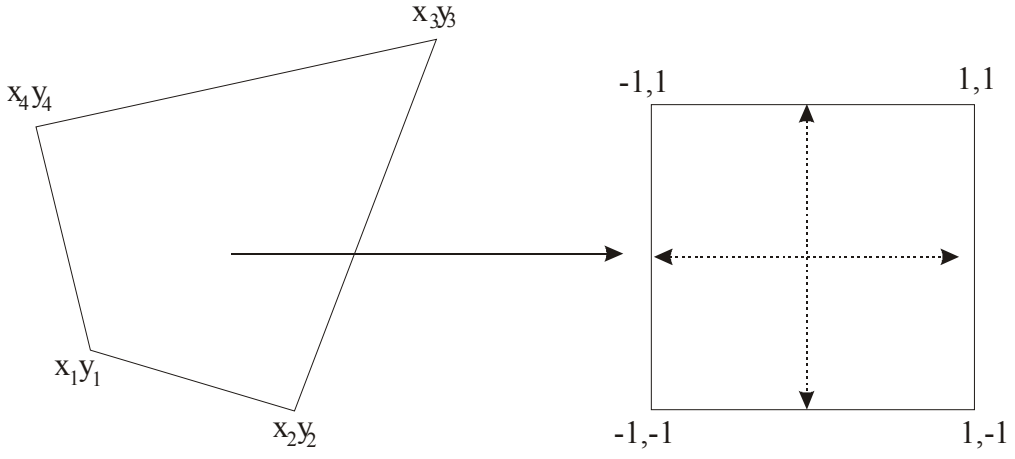


Figure 14-1: Warped element transformed to a Isoparametric element.

The Jacobian of the four Gauss points is different for each point. It is calculated as Eq. (14.2), Eq. (14.3) and Eq. (14.4). Eq. (14.4) gives the equations and factors for use in the shape function. The value r_i or s_i is taken from the accompanying table, the values of r and s are the coordinates of the Gauss point in question.

$$[J] = \begin{bmatrix} J_{11} & J_{12} \\ J_{21} & J_{22} \end{bmatrix} \qquad \text{Eq. (14.2)}$$

$$[J] = \begin{bmatrix} \frac{\delta N_1}{\delta r} & \cdots & \frac{\delta N_n}{\delta r} \\ \frac{\delta N_1}{\delta s} & \cdots & \frac{\delta N_n}{\delta s} \end{bmatrix} \begin{bmatrix} x_1 & y_1 \\ \vdots & \vdots \\ x_n & y_n \end{bmatrix} \qquad \text{Eq. (14.3)}$$

$$\begin{aligned} N_i &= \frac{1}{4}(1 + r_i r)(1 + s_i s) \\ \frac{dN_i}{dr} &= (r_i)(1 + s_i s) \\ \frac{dN_i}{dr} &= (s_i)(1 + r_i r) \end{aligned} \qquad \text{Eq. (14.4)}$$

i	1	2	3	4
r_i	−1	1	1	−1
s_i	−1	−1	1	1

The value of the function is calculated at each of these Gauss points and then over the determinate and Jacobian returned to the normal coordinate system. This is illustrated in Figure 14-2, and may be found in the accompanying excel sheet. Refering to Kolditz 2001, the equation notation is repeated here for clarity under „Terms“. The conductance matrix is the sum of the four contributions, as each contribution is awarded the weight of 1 in a two point guass system per dimension.

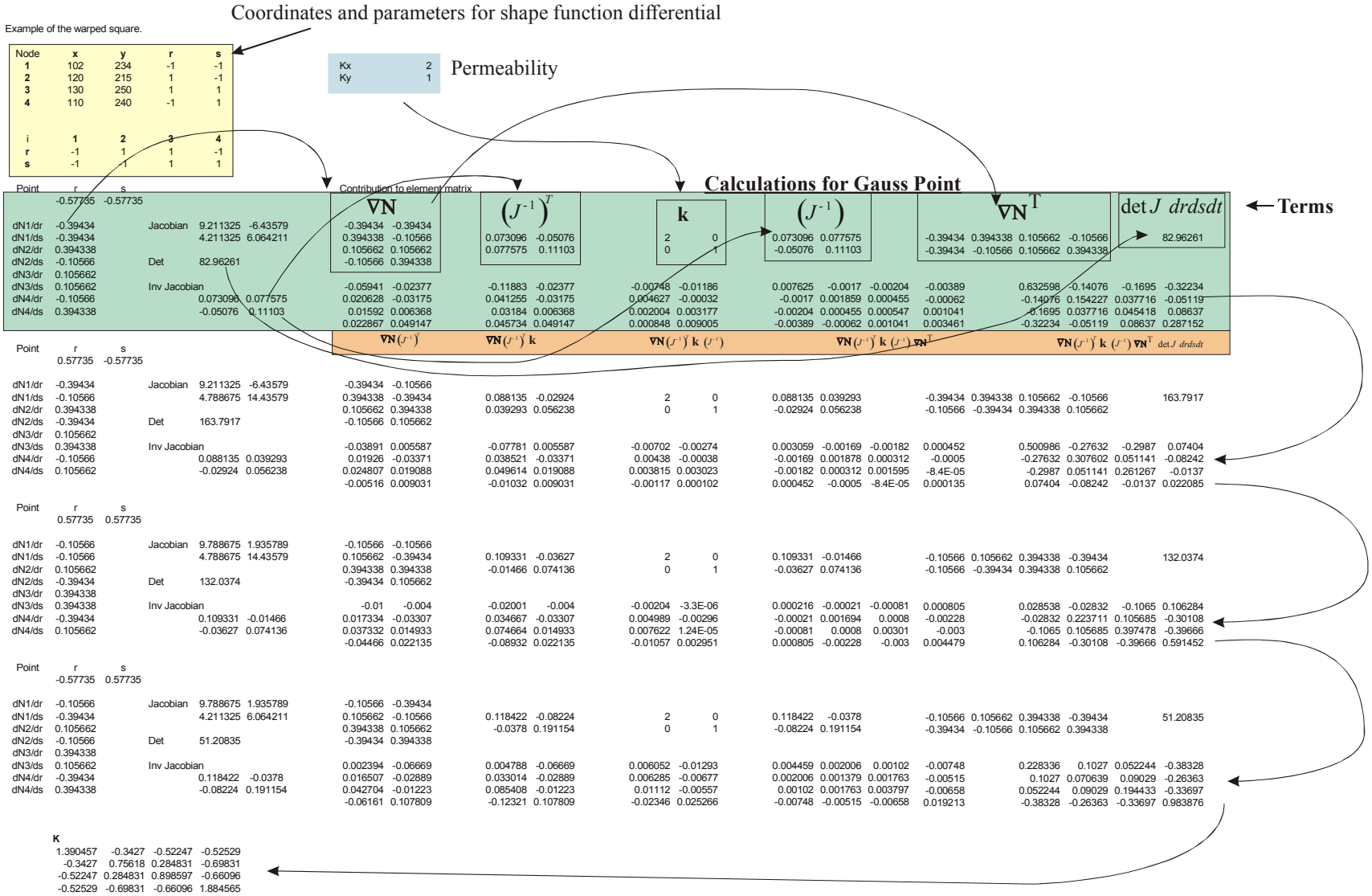


Figure 14-2: Warped element transformed to local co-ordinate system and then back to global co-ordinate system.

15. Coordinate Transformation: Local coordinates to global coordinates.

Last but not lest is understanding the origin of the matrix T for the coordinate transformation. Here in Kolditz 2001 we have the permeability presented as $T^T kT$.

In the section on Stress Strain Analysis we derived the formulation

$$\begin{bmatrix} \bar{u}_{xi} \\ \bar{u}_{yi} \\ \bar{u}_{xj} \\ \bar{u}_{yi} \end{bmatrix} = \begin{bmatrix} c & s & 0 & 0 \\ -s & c & 0 & 0 \\ 0 & 0 & c & s \\ 0 & 0 & -s & c \end{bmatrix} \begin{bmatrix} u_{xi} \\ u_{yi} \\ u_{xj} \\ u_{yi} \end{bmatrix} \qquad \text{Eq. (15.1)}$$

Here the 4 x 4 matrix is the transformation matrix. This changes the global coordinate movements into local coordinate movements and vice versa.

Considering permeability
The co-ordinate transformation is given by (2D):-

$$\begin{pmatrix} x' \\ y' \end{pmatrix} = \begin{pmatrix} \cos\beta & \sin\beta \\ -\sin\beta & \cos\beta \end{pmatrix} \begin{pmatrix} x \\ y \end{pmatrix} \qquad \text{Eq. (15.2)}$$

$$T = \begin{pmatrix} \cos\beta & \sin\beta \\ -\sin\beta & \cos\beta \end{pmatrix} \qquad \text{Eq. (15.3)}$$

Now $q = -K\nabla h$ From Eq. (15.3) we have $q' = Tq$. Also $(\nabla h)' = T(\nabla h)$. Therefore $Tq = -K'T\nabla h$ and finally

$$q = \underbrace{-T^T K' T}_{K} \nabla h \qquad \text{Eq. (15.4)}$$

For stress and strain we get

$$T = \begin{bmatrix} \cos^2\beta & \sin^2\beta & -2\sin\beta\cos\beta \\ \sin^2\beta & \cos^2\beta & 2\sin\beta\cos\beta \\ \sin\beta\cos\beta & -\sin\beta\cos\beta & \cos^2\beta - \sin^2\beta \end{bmatrix} \qquad \text{Eq. (15.5)}$$

This is not trivial to derive, and includes considering forces and resolving them, then rotating the axis.

$$\sigma_{x'} = \sigma_x \cos^2\theta + 2\tau_{xy}\sin\theta\cos\theta + \sigma_y \sin^2\theta \qquad \text{Eq. (15.6)}$$

$$\sigma_{y'} = \sigma_x \sin^2\theta - 2\tau_{xy}\cos\theta\sin\theta + \sigma_y \cos^2\theta \qquad \text{Eq. (15.7)}$$

$$\tau_{x'y'} = (\sigma_y - \sigma_x)\sin\theta\cos\theta + \tau_{xy}(\cos^2\theta - \sin^2\theta) \qquad \text{Eq. (15.8)}$$

Allowing D to describe

$$\boldsymbol{\sigma = D\varepsilon} \qquad \text{Eq. (15.9)}$$

Then in the applying local and global coordinate systems we have

$$\mathbf{D = T^T D' T} \qquad \text{Eq. (15.10)}$$