Numerical Approximation Methods - 1D

1. Problem Description

1.1 Groundwater Flow 1D

The 1D groundwater flow problem can be described for a confined situation by:

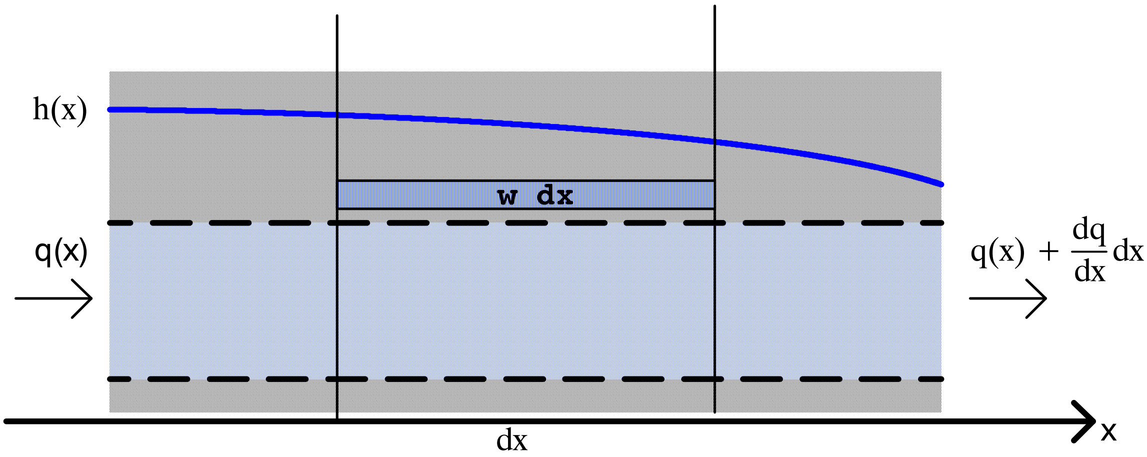

Figure 1: Groundwater 1D flow in a differential element

q(x)	groundwater flux in coordinate direction
h(x)	hydraulic head
w(x)	external extraction/injection flux
x	1D coordinate
dx	length of a “small” control (differential) element

The groundwater 1D confined flow problem has two main physical state variables: hydraulic (potentiometric, piezometric) head h(x) and the groundwater flux q(x). Darcy‘s law is used in this lecture notes as material law using the hydraulic conductivity as material constant. External extraction or injection flux will be considered as constant over specified model domain regions. Boundary conditions for head or flux are specified at each end of the model domain.

1.2 Mathematical Description

Differential Equation

The groundwater problem can be describe by the set of differential equations for flow balance in the model domain and at the boundary of the model domain.

(1-1) $$\frac{\partial}{\partial x_1}\left[K_{11}\frac{\partial h}{\partial x_1}\right] + \frac{\partial}{\partial x_2}\left[K_{22}\frac{\partial h}{\partial x_2}\right] + \frac{\partial}{\partial x_3}\left[K_{33}\frac{\partial h}{\partial x_3}\right] + w = S_s\frac{\partial h}{\partial t}$$

K_{11}, K_{22}, K_{33}	hydraulic conductivity along x_i coordinate
h	hydraulic head
w	volumetric flux (source/sink term)
S_s	specific storage of the soil material (porous material)
x_1, x_2, x_3	Cartesian coordinates
t	time coordinate

For 1D problems with constant hydraulic conductivity the equation can be simplified to:

(1-2) $$K\frac{\partial^2 h}{\partial x^2} + w = S_s\frac{\partial h}{\partial t}$$

For steady groundwater flow the equation can be simplified to:

(1-3) $$K\frac{\partial^2 h}{\partial x^2} + w = 0$$

The groundwater flux is defined by:

(1-4) $$q = -K\frac{\partial h}{\partial x}$$

Boundary conditions:

(1-5)	$h = h_0$	Dirichlet boundary condition, given head
(1-6)	$q = q_0$	Neumann boundary condition, given flux
(1-7)	$q = f(h)$	Cauchy boundary condition, flux depends on head

Integral Equation

The integral equation of the groundwater problem can be obtained in two ways. First option is to set up the potential for the whole model domain. Based on the assumption of a conservative potential, the variation of the potential is zero. The other option is the method of weighted residuals. In case of an approximation of the physical state variables, the specified differential equations are not any more exactly accurate, a residual ε occurs. Example for equation (1-3):

(1-8) $$K\frac{\partial^2 h}{\partial x^2} + w = \epsilon$$

The method of weighted residuals weighted these residuals of all differential equations including the boundary conditions. The weighted residuals are integrated over the whole model domain and in total set to 0. Using the weighting method of Galerkin the integral equation (given head left side, given flux right side) can be specified by:

(1-9) $$\int_0^L \delta h\left(K\frac{\partial^2 h}{\partial x^2} + w\right)dx + \delta q(h_0 - h)\,|_0 + \delta h(q_L - q)\,|_L = 0$$

The first term of equation (1-9) can be transformed using the Green-Gauss Integral Theorem:

(1-10) $$\int_0^L \delta h\left(K\frac{\partial^2 h}{\partial x^2}\right)dx = -\int_0^L \delta\frac{\partial h}{\partial x}\left(K\frac{\partial h}{\partial x}\right)dx + \delta h\left(K\frac{\partial h}{\partial x}\right)\Big|_0^L$$

Using this transformation equation (1-9) can be expressed by:

(1-11) $$\int_0^L \delta\frac{\partial h}{\partial x}\left(K\frac{\partial h}{\partial x}\right)dx = \int_0^L \delta h \; w \; dx$$
$$+ \delta q(h_0 - h)\,|_0 - \delta h\left(K\frac{\partial h}{\partial x}\right)\Big|_0 + \delta h(q_L)\,|_L$$

This equation is valid for any variation of δh and δq.

1.3 Numerical Approximation Methods

The given boundary value problem can be solved by numerical methods. Three types of numerical approximation methods will be introduced:

- Finite Difference Method (FDM)
- Finite Element Method (FEM)
- Finite Volume Method (FVM)

The model domain is subdivided in small finite approximation objects, such as sections, cells or elements for all three methods. Nodes are introduced to specify the geometry of the model domain and to specify the topology of the approximation objects.

The Finite Difference Method is based on a setting up equations at the nodes within the model domain. At each node, the differential equation is solved exactly by related numerical difference quotients. The FDM requires structured grids.

The Finite Element Method is based on setting up equations within small finite elements. For each element a related integral equation is set up and combined to equations for the whole system. This set of integral equations is minimized towards the approximation error in the whole model domain. In this way the Finite Element Method guarantees a global conservation of the related equations. The FEM can be used for unstructured meshes.

The Finite Volume Method is based on setting up equations on control volumes for each node or cell within the model domain. The balance equation of all control volumes is set up and combined towards a system of equations for the whole model domain to be solved. In this way the Finite Volume Method guarantees a local conservation of the related equations. The FVM can be used for unstructured meshes.

Method	Approximation Object	Equation
FDM	node	differential equation
FEM	element	integral equation
FVM	control volume	volume balance equation

2. Finite Difference Method FDM

2.1 Spatial Approximation of the domain

The model domain is subdivided into equidistant sections and related nodes:

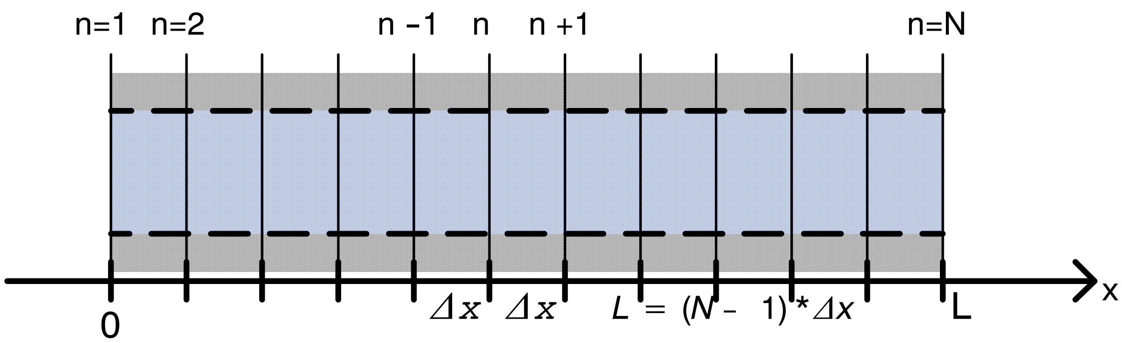

Figure 2: Introduction of equidistant nodes

The physical state variables h(x) and q(x) are described by discrete functions. At each node n the related function values h_n and q_n are specified.

2.2 Approximation of the Differential Equation

The groundwater 1D differential equation is a Laplace's equation. To solve this equation the order of an approximation polynomial for h(x) has to be two as minimum. The physical state variable h(x) is described by a shape function with three nodes (see lecture notes - Geometrical Modeling - Shape Functions). For each node n the related element starts from node n-1 and ends at node n+1 with an element length of $2\Delta x$.

(2-1) $$\frac{\partial^2 h}{\partial x^2} = \frac{1}{\Delta x^2} \boldsymbol{S}_{zze}^T \boldsymbol{h}_e$$

(2-2) $$\boldsymbol{s}_{zze} = \begin{bmatrix} 1 \\ -2 \\ 1 \end{bmatrix}$$ shape function 2nd derivation vector

(2-3) $$\boldsymbol{h}_e = \begin{bmatrix} h_{n-1} \\ h_n \\ h_{n+1} \end{bmatrix}$$ head value vector at node n

(2-4) $$-\frac{K}{\Delta x^2} \boldsymbol{s}_{zze}^T \boldsymbol{h}_e = w_n$$ approximated diff. equation at node n

(2-5) $$w_n = w(x)$$

w_n flux load at node n

The final equation for the differential equation at node n is:

(2-6) $$\frac{K}{\Delta x^2}(-h_{n-1} + 2h_n - h_{n+1}) = w_n$$

Taylor Series

Instead of shape functions, the approximation of the head function can be also done by taylor series analysis:

forward

(2-7) $$h(x+\Delta x) = h(x) + \Delta x \frac{dh}{dx} + \frac{\Delta x^2}{2}\frac{d^2h}{dx^2} + \frac{\Delta x^3}{6}\frac{d^3h}{dx^3} + \ldots$$

backward

(2-8) $$h(x-\Delta x) = h(x) - \Delta x \frac{dh}{dx} + \frac{\Delta x^2}{2}\frac{d^2h}{dx^2} - \frac{\Delta x^3}{6}\frac{d^3h}{dx^3} + \ldots$$

sum of forward and backward

(2-9) $$h(x-\Delta x) + h(x-\Delta x) = 2h(x) + \Delta x^2 \frac{d^2h}{dx^2} + \ldots$$

(2-10) $$\frac{d^2h}{dx^2} = \frac{h_{n-1} - 2h_n + h_{n+1}}{\Delta x^2}$$

This is equal to equation as (2-1) derived from the shape function concept.

2.3 Approximation of the Boundary Conditions

Two boundary conditions types are considered for the 1D groundwater flow approximation: given head values and given flux values.

Given head values can be directly set to the related node values

(2-11) $h(x=0) = h_0$ left

(2-12) $h(x=L) = h_L$ right

The groundwater flux is specified by a differential equation, which can be approximated by a linear approach (see lecture noted geometrical modeling - shape functions). Depending on the left or right boundary two approximation equations are used:

(2-13) $$q(x) = -K\frac{\partial h}{\partial x} = \frac{-K}{\Delta x}\, \boldsymbol{s}_{ze}^T\, \boldsymbol{h}_e$$

(2-14) $$q(x=0) = q_0 = \frac{-K}{\Delta x}(h_2 - h_1) \qquad \text{left}$$

(2-15) $$q(x=L) = q_L = \frac{-K}{\Delta x}(h_N - h_{N-1}) \qquad \text{right}$$

(2-16) $$\boldsymbol{s}_{ze} = \begin{bmatrix} -1 \\ 1 \end{bmatrix}$$ shape function 1st derivation vector

(2-17) $$\boldsymbol{h}_e = \begin{bmatrix} h_{n-1} \\ h_n \end{bmatrix}$$ head value vector at node n

The left boundary condition has a surface normal of |-1| (flux outflow in opposite to the coordinate direction).

2.4 Equation system

The groundwater flow system in Figure 2 is approximated at each node. The given boundary conditions at the nodes n=1 and n= N are approximated by one equation each. For each inner node n=2 to n=N-1 the groundwater flow differential equation is approximated. This leads to N equations with N unknown values (h_n).

The N equations can be written in a matrix - vector notation. The unknown head values are summarized in the vector **h**. The known external flux w(x) will be lumped to the node location and summarized in the load vector **w**. The coefficients related to the unknown head values at each node are considered in a system matrix.

(2-18) $$\boldsymbol{Kh} = \boldsymbol{w}$$

(2-19) $$\boldsymbol{K} = \frac{K}{\Delta x^2} \begin{bmatrix} \frac{\Delta x^2}{K} & 0 & & & & \\ -1 & 2 & -1 & \ldots & & \\ & \ldots & -1 & 2 & -1 & \ldots \\ & & \ldots & -1 & 2 & -1 \\ & & & & \Delta x & -\Delta x \end{bmatrix}$$

K system matrix (left boundary given head, right boundary given flux)

(2-20) $$\boldsymbol{h} = \begin{bmatrix} h_1 \\ \ldots \\ h_n \\ \ldots \\ h_N \end{bmatrix}$$ (unknown) head vector

(2-21) $$\boldsymbol{w} = \begin{bmatrix} h_0 \\ w_2 \\ \ldots \\ w_n \\ \ldots \\ w_{N-1} \\ q_L \end{bmatrix}$$ (known) external load vector

3. Finite Volume Method - FVM

3.1 Spatial Approximation of the domain

The model domain is subdivided into equidistant sections/cells and related nodes:

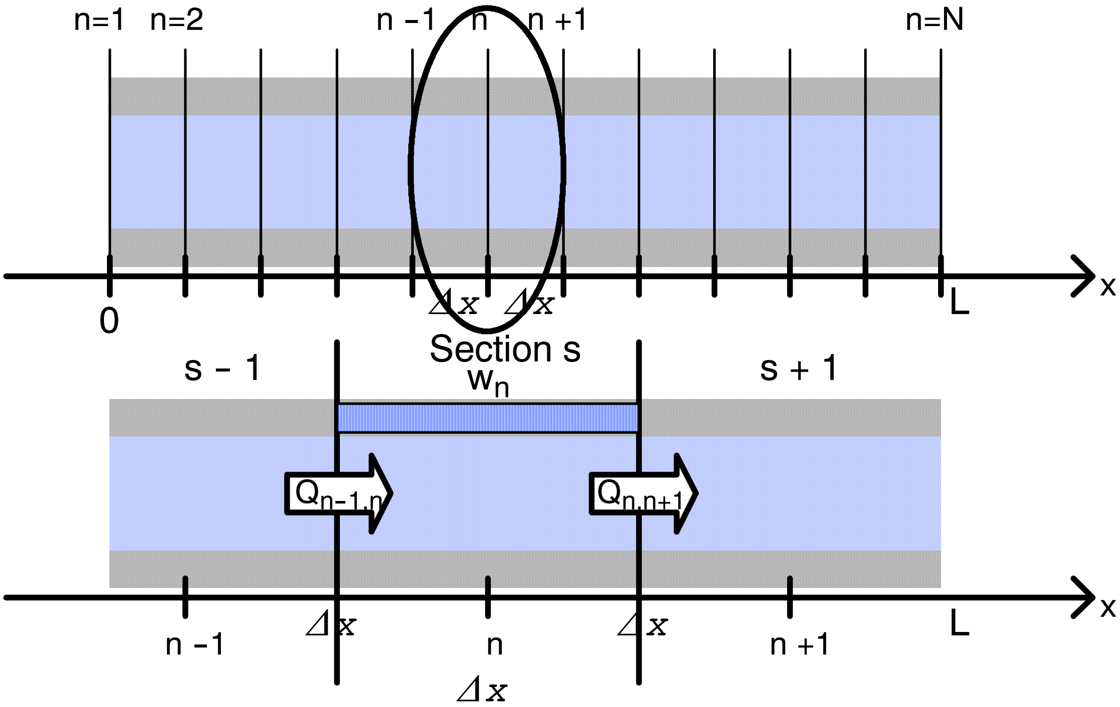

Figure 3: Introduction of sections and nodes

The physical state variables h(x) and q(x) are described by discrete functions. At each node n the related function values h_n and q_n are specified.

3.2 Approximation of the Balance Equation

For each section/cell the local flux balance is defined by:

(3-1) $$Q_{n-1,n} - Q_{n,n+1} + w_n \Delta x = 0$$

The area of the model domain volume cell at the left and right side are the same. Instead of Q and W the related physical state variables q and w for a normalized area 1 can be used. Using Darcy's law for the flow across the section/cell boundary:

(3-2) $$q_{i-1,i} = -K\frac{h_i - h_{i-1}}{\Delta x}$$

this leads to the approximation equation

(3-3) $$-K\frac{h_{n-1} - h_n}{\Delta x} + K\frac{h_n - h_{n+1}}{\Delta x} + w_n \Delta x = 0$$

$$\frac{K}{\Delta x^2}\left(-h_{n-1} + 2h_n - h_{n+1}\right) = w_n$$

For this specific problem the final equation is the same equation as (2-6) for the Finite Difference Method and leads to the same equation system.

4. Finite Element Method - FEM

4.1 Spatial Approximation of the domain

The model domain is subdivided into equidistant elements and related nodes:

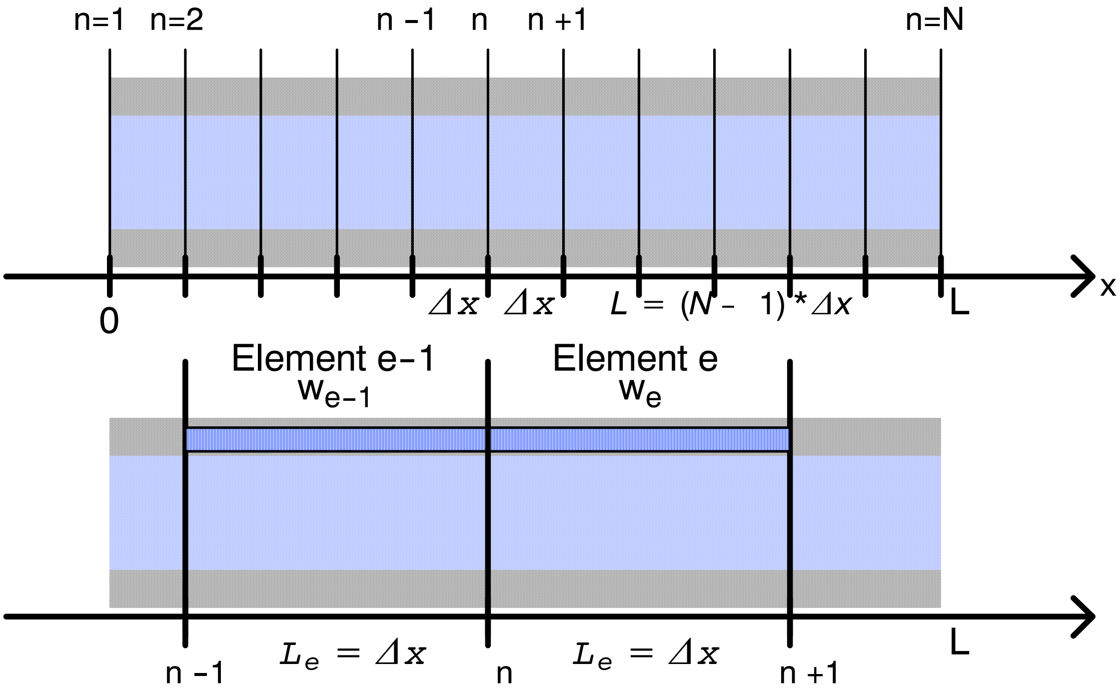

Figure 4: Introduction of elements and nodes

The physical state variables h(x) and q(x) are described by discrete functions. At each node n the related function values h_n and q_n are specified.

4.2 Approximation of the Integral Equation

Element Functions

For each element in the model domain the unknown physical state variable h(x) will be described by suitable shape functions. The integral equation contains the gradient of h(x), a linear shape function approximation of degree 1 is requested.

(4-1) $$h_e(x) = \boldsymbol{s}_e^T \boldsymbol{h}_e$$

(4-2) $$\boldsymbol{s}_e = \begin{bmatrix} \frac{1}{2}(1 - z) \\ \frac{1}{2}(1 + z) \end{bmatrix}$$ shape function vector

(4-3) $$\boldsymbol{h}_e = \begin{bmatrix} h_e \\ h_{e+1} \end{bmatrix}$$ element head vector

The differentiation of (1-6) leads to:

(4-4) $$\frac{\partial h_e(x)}{\partial x} = \det \boldsymbol{Z}_x \; \boldsymbol{s}_{ez}^T \boldsymbol{h}_e = \frac{2}{L_e} \boldsymbol{s}_{ez}^T \boldsymbol{h}_e$$

(4-5) $$\det \boldsymbol{Z}_x = \frac{2}{L_e}$$

(4-6) $$\boldsymbol{s}_{ze} = \begin{bmatrix} -\frac{1}{2} \\ \frac{1}{2} \end{bmatrix}$$ shape function derivation vector

System Approximation

The physical state variable head within the model domain is described by a discrete scalar function as described in the lecture notes for geometry modelling - shape functions.

(4-7) $$h(x) = \sum_{e=1}^{E} g_e h_e(x) = \sum_{e=1}^{E} g_e \boldsymbol{s}_e^T \boldsymbol{h}_e$$

(4-8) $$g_e = \begin{matrix} 0 & x \le x_e, x > x_{e+1} \\ 1 & x_e < x \le x_{e+1} \\ 1 & e = 1, x = x_{e+1} \end{matrix}$$

The function value for h(x) at the right element boundary node n is equal to the function value at the element boundary of the next element, as this boundary is defined by the same node n. Similar statement is given for the left boundary at node n-1 and the last element. The function values at all nodes are combined to a system vector **h**.

(4-9) $$\boldsymbol{h} = \begin{bmatrix} h_1 \\ \cdots \\ h_n \\ \cdots \\ h_N \end{bmatrix}$$ system head vector

The relationship between the element head vector and the system head vector can be specified by a reduction matrix [2,N], with one value 1. per row.

(4-10) $$\boldsymbol{h}_e = \boldsymbol{R}_e \boldsymbol{h}$$ element-system relationship

The head variable and related derivative can be expressed by:

(4-11) $$h(x) = \sum_{e=1}^{E} (\boldsymbol{s}_e^T \boldsymbol{R}_e) \; \boldsymbol{h} = \boldsymbol{h}^T \sum_{e=1}^{E} (\boldsymbol{R}_e^T \boldsymbol{s}_e)$$

(4-12) $$\frac{\partial h}{\partial x} = \sum_{e=1}^{E} (\det \boldsymbol{Z}_x \boldsymbol{s}_{ze}^T \boldsymbol{R}_e) \boldsymbol{h} = \boldsymbol{h}^T \sum_{e=1}^{E} (\boldsymbol{R}_e^T \boldsymbol{s}_{ze} \det \boldsymbol{Z}_x)$$

Similar equations can be set up for the variation of head and head gradient. The head function value of each node is independent, this leads to N equations for the variations:

(4-13) $$(\delta h)_n = \sum_{e=1}^{E} (\boldsymbol{s}_e^T \boldsymbol{R}_e) \ \boldsymbol{i}_n = \boldsymbol{i}_n^T \sum_{e=1}^{E} (\boldsymbol{R}_e^T \boldsymbol{s}_e)$$

(4-14) $$\delta\left(\frac{\partial h}{\partial x}\right)_n = \sum_{e=1}^{E} (det \boldsymbol{Z}_x \boldsymbol{s}_{ze}^T \boldsymbol{R}_e) \boldsymbol{i}_n = \boldsymbol{i}_n^T \sum_{e=1}^{E} (\boldsymbol{R}_e^T \boldsymbol{s}_{ze} \det \boldsymbol{Z}_x)$$

The integral equation (1-11) is used for the Finite Element Method. The boundary conditions specified by given head values are explicitly considered.

(4-15) $$\int_0^L \delta \frac{\partial h}{\partial x}\left(K \frac{\partial h}{\partial x}\right) dx = \int_0^L \delta h \ w \ dx - \delta h\left(K \frac{\partial h}{\partial x}\right)\Big|_0 + \delta h(q_L)\Big|_L$$

Using the approximation equations (4-11) to (4-14):

(4-16) $$\int_0^L \sum_{e=1}^{E} \boldsymbol{i}_n^T \ \boldsymbol{R}_e^T \boldsymbol{s}_{ze} K_e \boldsymbol{s}_{ze}^T \boldsymbol{R}_e \frac{4}{L_e^2} \ \boldsymbol{h} dx = \int_0^L \sum_{e=1}^{E} \boldsymbol{i}_n^T \ \boldsymbol{R}_e^T \boldsymbol{s}_e \ w_e \ dx$$
$$+ q\big|_{n=1} + q_L\big|_{n=N} \qquad n = 1, ..., N$$

The n equations can be combined in a linear equation system:

(4-17) $$\boldsymbol{K}\boldsymbol{h} = \boldsymbol{w} + \boldsymbol{q}$$

(4-18) $$\boldsymbol{K} = \sum_{e=1}^{E} \int_0^{L_e} \boldsymbol{R}_e^T \boldsymbol{s}_{ze} \frac{4}{L_e^2} K_e \boldsymbol{s}_{ze}^T \boldsymbol{R}_e dx = \sum_{e=1}^{E} \boldsymbol{R}_e^T \boldsymbol{K}_e \boldsymbol{R}_e$$

(4-19) $$\boldsymbol{w} = \sum_{e=1}^{E} \int_0^{L_e} \boldsymbol{R}_e^T \boldsymbol{s}_e w_e = \sum_{e=1}^{E} \boldsymbol{R}_e^T \boldsymbol{w}_e$$

(4-20) $$\boldsymbol{q} = \begin{bmatrix} q_1 \\ 0 \\ \cdots \\ 0 \\ q_N \end{bmatrix}$$ external reaction

The integral over the model domain is transferred to a sum over element integrals.

4.3 Element Matrix and Vector

Element matrix and element vector can be determined using the shape function integration methods (e.g. Gaussian integration).

(4-21) $$\boldsymbol{K}_e = \int^{L_e} K_e \ \det \boldsymbol{Z}_x \ \boldsymbol{s}_{ez} \boldsymbol{s}_{ez}^T \det \boldsymbol{Z}_x dx = \frac{K_e}{L_e} \begin{bmatrix} 1 & -1 \\ -1 & 1 \end{bmatrix}$$

(4-22) $$\boldsymbol{w}_e = \int^{L_e} w \ \boldsymbol{s}_e \ dx = w \ L_e \begin{bmatrix} \frac{1}{2} \\ \frac{1}{2} \end{bmatrix}$$

4.4 Equation System

The system approximation and the boundary condition for given head values leads to a linear equation system:

(4-23) $$\boldsymbol{K}\boldsymbol{h} = \boldsymbol{w}$$

According to equation (4-18) and (4-19) the system matrix **K** and the system vector **w** is summed up by the related element components (example constant k and Δx):

(4-24) $$\boldsymbol{K} = \frac{K}{\Delta x} \begin{bmatrix} \frac{\Delta x}{K} & 0 & & & & \\ -1 & 1+1 & -1 & \dots & & \\ \dots & -1 & 1+\mathbf{1} & -\mathbf{1} & & \dots \\ & \dots & -\mathbf{1} & \mathbf{1}+1 & -1 & \\ & & & 1 & -1 & \end{bmatrix}$$

K system matrix (left boundary given head, right boundary given flux)
bold elements are contributions of one element

(4-25) $$\boldsymbol{h} = \begin{bmatrix} h_1 \\ \dots \\ h_n \\ \dots \\ h_N \end{bmatrix}$$ (unknown) head vector

(4-26) $$\boldsymbol{w} = \begin{bmatrix} h_1 \\ w_2 \\ \dots \\ w_n \\ \dots \\ w_{N-1} \\ q_L \end{bmatrix}$$ (known) external load vector

For this specific problem the final equation system of the Finite Element Method is the same as for the Finite Difference Method (factor Δx).