

Lecture Modelling of Hydro-systems Mass Transport Process Part II

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Basics of Finite Element Method



0.9998

0.9000 0.8000 0.7000

0.6000

0.5000

0.3000

0.2000

0.0000

x (m)

Finite element in space

The numerical method of FEM employs the <u>Method of Weighted Residuals (MWR)</u> to find the solution of a PDE.

MWR can be divided into 3 steps:

- Approximation of the unknown function by a trial solution;
- 2) Definition of weighting functions;
- 3) Derivation of a system of algebraic equations, and solve it to find the approximation solution.



$$\frac{\partial}{\partial t}u + \nabla \cdot \Phi^u = q^u$$

Let Φ^u be the flux vector of conservative quantity u and q^u the source/sink term (see our first lecture about GROUNDWATER_FLOW process)

Applying the approximation, we get the weak form of the above equation as

$$\int_{\Omega} \omega_i \frac{\partial u}{\partial t} d\Omega + \int_{\Omega} \omega_i \nabla \cdot \Phi^u d\Omega = \int_{\Omega} \omega_i q^u d\Omega$$

In order to get rid of the special derivative of flux term, we apply the Green's theorem

$$\int_{\Omega} \omega_i \frac{\partial u}{\partial t} d\Omega - \int_{\Omega} \Phi^u \cdot \nabla \omega_i d\Omega + \oint_{\partial \Omega} \omega_i \Phi^u dS = \int_{\Omega} \omega_i q^u d\Omega$$

Finite element in space



So that the above equation becomes

$$\sum_{i} \frac{du_{j}}{dt} \int_{\Omega} \omega_{i} \omega_{j} d\Omega - \sum_{i} \Phi^{u} \cdot \int_{\Omega} \omega_{j} \nabla \omega_{i} d\Omega + \oint_{\partial \Omega} \omega_{i} \Phi^{u} dS = \int_{\Omega} \omega_{i} q^{u} d\Omega$$

$$M_{ij} = \int_{\Omega} \omega_{i} \omega_{j} d\Omega \qquad K_{ij} = \int_{\Omega} \omega_{j} \nabla \omega_{i} d\Omega$$
This part is applied on element Mass Matrix
"shape-shape"
This part is applied on element Stiffness Matrix
This part should zero out.
"When time is infinitely short, how much flowing-in should equal to how much flowing-out"

Shape functions (1D line element)

true solution U(X)First let's explore how the shape function is calculated for a 1D line element. approximate A simple approximation of the unknown functio u(x) can solution be obtained by linear approximation. $\hat{u}(x) = a_1 + a_2 x$ \mathbf{X}_2 X₁ On the two ends of the line element, we assume that our Inknown function produces u1 and u2 at position x1 and x2. $u_1 = a_1 + a_2 x_1$ $\left(\begin{array}{c} u_1 \\ u_2 \end{array}\right) = \left|\begin{array}{c} 1 & x_1 \\ 2 & x_2 \end{array}\right| \left(\begin{array}{c} a_1 \\ a_2 \end{array}\right)$ Write in a linear algebra form $u_2 = a_1 + a_2 x_2$ Make an inversion of the expression, we get the a1 and a2 value dependency on u1 and u2. $\begin{pmatrix} a_1 \\ a_2 \end{pmatrix} = \frac{1}{x_2 - x_1} \begin{bmatrix} x_2 & -x_1 \\ -1 & 1 \end{bmatrix} \begin{pmatrix} u_1 \\ u_2 \end{pmatrix}$ Wirte back to the standard form $a_1 = \frac{1}{x_2 - x_1} (x_2 u_1 - x_1 u_2)$ Insert back here $a_2 = \frac{1}{x_2 - x_1} (-u_1 + u_2)$ Then we get the expression of approximated solution based on the location

$$\hat{u}(x) = \frac{x_2 - x}{x_2 - x_1} u_1 + \frac{x - x_1}{x_2 - x_1} u_2 = N_1(x) u_1 + N_2(x) u_2$$

N1(x) and N2(x) are the so-called shape functions.

Shape functions (1D line element, higher orders)

Linear

Approximation

$$\hat{u}(x) = a_1 + a_2 x$$

Shape Function

$$N_1(x) = \frac{x_2 - x}{x_2 - x_1}$$
$$N_2(x) = \frac{x - x_1}{x_2 - x_1}$$

$$\hat{u}(x) = a_1 + a_2 x + a_3 x^2$$

. .

$$N_1(x) = \frac{(x - x_2)(x - x_3)}{(x_1 - x_2)(x_1 - x_3)}$$
$$N_2(x) = \frac{(x - x_1)(x - x_3)}{(x_2 - x_1)(x_2 - x_3)}$$
$$N_2(x) = \frac{(x - x_1)(x - x_2)}{(x - x_1)(x - x_2)}$$

$$N_3(x) = \frac{(x - x_1)(x - x_2)}{(x_3 - x_2)(x_3 - x_1)}$$





Shape functions (2D line triangle element)

$$\hat{u}(x,y) = a_1 + a_2 x + a_3 y$$

The interpolation writes as

 $u_1 = a_1 + a_2 x_1 + a_3 y_1$ $u_2 = a_1 + a_2 x_2 + a_3 y_2$ $u_3 = a_1 + a_2 x_3 + a_3 y_3$

Write it in the matrix-vector form

ſ	u_1)		[1	x_1	y_1	11	a_1)
{	u_2		$\rightarrow =$	1	x_2	y_2	13	a_2	ł
l	u_3	J		$\lfloor 1$	x_3	y_3	J	a_3	J

Inversion of the above relationship will give

$$\left\{ \begin{array}{c} a_1\\ a_2\\ a_3 \end{array} \right\} = \frac{1}{2A} \left[\begin{array}{ccc} x_2y_3 - x_3y_2 & x_3y_1 - x_1y_3 & x_1y_2 - x_2y_1\\ y_2 - y_3 & y_3 - y_1 & y_1 - y_2\\ x_3 - x_2 & x_1 - x_3 & x_2 - x_1 \end{array} \right] \left\{ \begin{array}{c} u_1\\ u_2\\ u_3 \end{array} \right\}$$

With A the surface area of the triangle

$$A = \frac{1}{2} \begin{vmatrix} x_1 & y_1 & 1 \\ x_2 & y_2 & 1 \\ x_3 & y_3 & 1 \end{vmatrix}$$

So again our shape function act like

$$\hat{u}(x,y) = N_1(x,y)u_1 + N_2(x,y)u_2 + N_3(x,y)u_3$$

They can be explicitly calculated as

$$N_1(x,y) = \frac{1}{2A} \left[(x_2y_3 - x_3y_2) + (y_2 - y_3)x + (x_3 - x_2)y \right]$$
$$N_2(x,y) = \frac{1}{2A} \left[(x_3y_1 - x_1y_3) + (y_3 - y_1)x + (x_1 - x_3)y \right]$$
$$N_3(x,y) = \frac{1}{2A} \left[(x_1y_2 - x_2y_1) + (y_1 - y_2)x + (x_2 - x_1)y \right]$$

Or in the matrix vector form

$$\left\{ \begin{array}{c} N_1\\N_2\\N_3 \end{array} \right\} = \frac{1}{2A} \left[\begin{array}{cccc} x_2y_3 - x_3y_2 & y_2 - y_3 & x_3 - x_2\\ x_3y_1 - x_1y_3 & y_3 - y_1 & x_1 - x_3\\ x_1y_2 - x_2y_1 & y_1 - y_2 & x_2 - x_1 \end{array} \right] \left\{ \begin{array}{c} 1\\x\\y \end{array} \right\}$$



Finite difference in time

We start from the mass transport governing equation



Source and Rink Term, i.e. decay and reaction

- Make a difference of previous and current time step value for primary unknown.
- For the time discretization part, we use \geq forward Euler method:
- For all C values in the spatial discretization part, we apply linear interpolation btw previous and current values:

 C^n – previous time step value C^{n+1} – current time step value $\frac{\partial C}{\partial t} = \frac{C^{n+1} - C^n}{\Lambda t}$

$$C = (1 - \theta)C^n + \theta C^{n+1}$$

- θ = 1 : C taken from the current time step, AKA implicit scheme.
- θ = 0 : C taken from the previous time step, AKA explicit scheme.

Finite difference in time



Handle the time derivative

We know all the previous time step value, so keep known things to the RHS and unknown things to the other.

Handle the space derivative

$$\frac{1}{\Delta t}C^{n+1} + \nabla(-D \cdot \nabla\theta C^{n+1}) + v \cdot \nabla(\theta C^{n+1})$$
$$= \frac{1}{\Delta t}C^n - (\nabla(-D \cdot \nabla(1-\theta)C^n) + v \cdot \nabla((1-\theta)C^n)) + Q$$

 $\text{Mass Term} \qquad \frac{1}{\Delta t} C^{n+1} \Rightarrow \int_{\Omega^e} \mathbf{N} \cdot C^{n+1} \cdot \mathbf{N} d\Omega \Rightarrow \int_{\Omega^e} \mathbf{N} \cdot \mathbf{N} d\Omega \cdot C^{n+1}$

$$\begin{array}{ll} \text{Dispersion/} & \nabla(-D\cdot\nabla(\theta C^{n+1})) \Rightarrow \int_{\Omega^e} \nabla \mathbf{N} \cdot (-D) \nabla \mathbf{N}^{\mathbf{T}} d\Omega^e \cdot \theta C^{n+1} \\ \text{Diffusion} & \end{array}$$

Advection

$$v \cdot \nabla(\theta C^{n+1}) \Rightarrow \int_{\Omega^e} \mathbf{N} \cdot (\theta v C^{n+1}) \nabla \mathbf{N}^{\mathbf{T}} d\Omega^e \Rightarrow \int_{\Omega^e} \mathbf{N} \cdot (v) \nabla \mathbf{N}^{\mathbf{T}} d\Omega^e \cdot \theta C^{n+1}$$

Handle the space derivative

$$\begin{split} & \frac{1}{\Delta t}C^{n+1} + \nabla(-D\cdot\nabla\theta C^{n+1}) + v\cdot\nabla(\theta C^{n+1}) \\ &= \frac{1}{\Delta t}C^n - (\nabla(-D\cdot\nabla(1-\theta)C^n) + v\cdot\nabla((1-\theta)C^n)) + Q \\ \\ & \text{Mass Term} \qquad \frac{1}{\Delta t}C^{n+1} \Rightarrow \int_{\Omega^e} \mathbf{N}\cdot C^{n+1}\cdot\mathbf{N}d\Omega \Rightarrow \underbrace{\int_{\Omega^e} \mathbf{N}\cdot\mathbf{N}d\Omega\cdot C^{n+1}}_{\mathbf{Mass Matrix}} \\ & \text{Dispersion/} \\ & \text{Dispersion/} \qquad \nabla(-D\cdot\nabla(\theta C^{n+1})) \Rightarrow \underbrace{\int_{\Omega^e} \nabla \mathbf{N}\cdot(-D)\nabla \mathbf{N}^{\mathbf{T}}d\Omega^e}_{\mathbf{Dispersion Matrix}} \\ & \text{Advection} \qquad v\cdot\nabla(\theta C^{n+1}) \Rightarrow \int_{\Omega^e} \mathbf{N}\cdot(\theta v C^{n+1})\nabla \mathbf{N}^{\mathbf{T}}d\Omega^e \Rightarrow \underbrace{\int_{\Omega^e} \mathbf{N}\cdot(v)\nabla \mathbf{N}^{\mathbf{T}}d\Omega^e}_{\mathbf{\Omega^e}} \cdot \theta C^{n+1} \end{split}$$

Advection Matrix

Handle the space
derivative
$$\frac{1}{\Delta t}C^{n+1} + \nabla(-D \cdot \nabla\theta C^{n+1}) + v \cdot \nabla(\theta C^{n+1}) \\
= \frac{1}{\Delta t}C^n - (\nabla(-D \cdot \nabla(1-\theta)C^n) + v \cdot \nabla((1-\theta)C^n)) + Q \\
= \frac{1}{\Delta t}C^n - (\nabla(-D \cdot \nabla(1-\theta)C^n) + v \cdot \nabla((1-\theta)C^n)) + Q \\
= \frac{1}{\Delta t}M \cdot C^{n+1} + Disp \cdot \theta C^{n+1} \\
= \frac{1}{\Delta t}M \cdot C^n + Disp \cdot (1-\theta)C^n + Adv \cdot (1-\theta)C^n + Q \\
= \frac{1}{\Delta t}M \cdot C^n + Disp \cdot (1-\theta)C^n + Adv \cdot (1-\theta)C^n + Q \\
= \frac{1}{\Delta t}M \cdot C^n + (Disp + Adv) \cdot \theta C^{n+1} \\
= \frac{1}{\Delta t}M \cdot C^n + (Disp + Adv) \cdot (1-\theta)C^n + Q \\
= \frac{1}{\Delta t}M \cdot C^n + (Disp + Adv) \cdot (1-\theta)C^n + Q \\
= \frac{1}{\Delta t}M \cdot C^n + (Disp + Adv) \cdot (1-\theta)C^n + Q \\
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= \frac{1}{\Delta t}M \cdot C^n + (Disp + Adv) \cdot (1-\theta)C^n + Q \\
= \frac{1}{\Delta t}M + (1-\theta)K) \cdot C^n + Q \\
= \frac{1}{\Delta t}M + (1-\theta)K \cdot C^n + Q \\
= \frac{1}{\Delta t}M + (1-\theta)K + C^n + Q \\
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= \frac{1}{\Delta t}M + (1-\theta)K + C^n + Q \\
= \frac{1}{\Delta t}M + (1-\theta)K + C^n + Q \\
= \frac{1}{\Delta t}M + Q \\
= \frac{1}{\Delta t}M$$

- -**Linear equation** Editor - E:\Google Drive\lectures TUD\matlab script ade fem\ade solver.m Text Go Cell Tools Debug Desktop Window Help File Edit assembly 🍓 🖅 🔹 🛤 🖛 🔿 filip 🕨 🛛 🛃 🔁 👘 👘 💷 🖓 🛄 filip 🦛 👘 የስ **P** 6 ⁺⊒ ⊑ × % % 0 - 1.0 +÷ 1.1 85 -= sparse(nn,nn); LHS 86 RHS = sparse(nn,1); 87 str = ['Time step ', num2str(ti), ' at time ', num2str(time steps(t: 88 disp(str); dt = time steps(ti+1) - time steps(ti); 89 $(\frac{1}{\Delta t}M + \theta K)C^{n+1}$ 90 % loop over all the elements, 91 for ie = 1 : ne92 % get the coordinates of connecting nodes $= \left(\frac{1}{\Lambda \star}M + (1-\theta)K\right) \cdot C^n + Q$ 93 sctr = elements(ie,:); 94 coord = nodes(sctr,:) ; 95 % local mass matrix 96 М = shapeshape tri(coord); % no coeff 97 % local advection matrix 98 -Adv = shapedshape tri(coord, [vel;0.0]);% % local dispersion/diffusion matrix 99 100 -Disp = dshapedshape tri(coord, [Dt, 0.0; 0.0, 0.01*Dt]); 101 % add advection and dispersion matrix t 102 -S = Adv + Disp; 103 % assemble to the LHS 104 l lhs= ((1.0/dt)*M + theta * S); 105 -LHS(sctr,sctr) = LHS(sctr,sctr) + 1 lhs; Ax = b106 % assemble to the RHS 107 -1 rhs= ((1.0/dt)*M - (1-theta)* S) * u pre(sctr); 108 -RHS(sctr) = RHS(sctr) + 1 rhs; 109 end 110 $\begin{bmatrix} a_{11} & a_{12} & a_{13} & \dots & a_{1n} \end{bmatrix} \begin{bmatrix} x_1 \end{bmatrix}$ - € 111 b 1 Ln 109 Col 8 script $\mathbf{a}_{21} \ \mathbf{a}_{22} \ \mathbf{a}_{23} \ \dots \ \mathbf{a}_{2n} \ \mathbf{x}_{2}$ b ,

 $\mathbf{a}_{31} \ \mathbf{a}_{32} \ \mathbf{a}_{33} \ \dots \ \mathbf{a}_{3} = |\mathbf{b}_{3}|$

1 b _m1

 $\begin{vmatrix} & \cdot & \cdot & \cdot & \cdot \\ \mathbf{a}_{m1} \mathbf{a}_{m2} \mathbf{a}_{m3} \cdots \mathbf{a}_{mn} \end{vmatrix} \mathbf{x}_{n}$

Linear equation assembly



$$\begin{bmatrix} a_{11} & a_{12} & a_{13} & \dots & a_{1n} \\ a_{21} & a_{22} & a_{23} & \dots & a_{2n} \\ a_{31} & a_{32} & a_{33} & \dots & \dots \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ a_{m1} & a_{m2} & a_{m3} & \dots & a_{mn} \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ \vdots \\ x_n \end{bmatrix} = \begin{bmatrix} b_1 \\ b_2 \\ b_3 \\ \vdots \\ b_m \end{bmatrix}$$

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-	+=	Ļ ⊒	-1.0 + $\div 1.1$ × $\%_{+}$ $\%_{-}$ 0											
	85	-	LHS = sparse(nn, nn);											
	86	-	RHS = sparse(nn,1);											
	87	-	<pre>str = ['Time step ', num2str(ti), ' at time ', num2str(time_steps(t</pre>											
	88	-	disp(str);											
	89	-	<pre>dt = time_steps(ti+1) - time_steps(ti);</pre>											
N	90		<pre>% loop over all the elements,</pre>											
	91	- [for ie = 1 : ne											
	92		<pre>% get the coordinates of connecting nodes</pre>											
	93	-	<pre>sctr = elements(ie,:);</pre>											
	94	-	<pre>coord = nodes(sctr,:) ;</pre>											
	95		<pre>% local mass matrix</pre>											
	96	-	<pre>M = shapeshape_tri(coord); % no coeff</pre>											
	97		<pre>% local advection matrix</pre>											
	98	-	Adv = shapedshape_tri(coord, [vel;0.0]);%											
	99		<pre>% local dispersion/diffusion matrix</pre>											
	100	-	<pre>Disp = dshapedshape_tri(coord, [Dt, 0.0; 0.0, 0.01*Dt]);</pre>											
	101		<pre>% add advection and dispersion matrix t</pre>											
	102	-	S = Adv + Disp;											
	103		% assemble to the LHS											
	104	-	l_lhs= ((1.0/dt)*M + theta * S);											
	105	-	LHS(sctr,sctr) = LHS(sctr,sctr) + 1_lhs;											
	106		% assemble to the RHS											
	107	-	l_rhs= ((1.0/dt)*M - (1-theta)* S) * u_pre(sctr);											
	108	-	RHS(sctr) = RHS(sctr) + 1_rhs;											
	109	-	- end											
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Impose Boundary Condition



Assuming we know the boundary value on one of the node, how can we solve the linear equation in a way that we get the desired value on this node?

The procedure is as follows:

- 1) Record the index of boundary node, say "i".
- 2) RHS vector minus the multiplication of fixed boundary node value with the i-th column of LHS matrix.
- 3) Record the i-th row and column entry value in LHS as TMP.
- 4) Make i-th row of LHS all zeros.
- 5) Make i-th column of LHS all zeros.
- 6) Overwrite i-th value in RHS vector as TMP times fixed boundary value
- Overwrite i-th row and column entry value in LHS matrix as xii.

Impose Boundary Condition

Taking the following linear equation as an example (represent a 1D Groundwater flow):



After imposing boundary nodes?



What result do you get by solving this linear equation system?

Peclet Number

Peclet number is defined as the ratio of the rate of advection to the rate of dispersion/diffusion.

 $Pe = \frac{vL}{D}$

Courant Number

AKA Courant–Friedrichs–Lewy condition

1D
$$Cr = \frac{v_x \Delta t}{\Delta x} \le Cr_{max}$$

2D
$$Cr = \frac{v_x \Delta t}{\Delta x} + \frac{v_y \Delta t}{\Delta y} \le Cr_{max}$$

- > Peclet number is dimensionless.
- Peclet number reflects the ratio of advection versus diffusion. If less than one, then diffusion dominated. If more than one, then advection dominated.
- Typically, the characteristic length L refers to the length of an element.
- For the accurate solution of finite element method, the Pe number has to be kept to be less than 2.

- > Courant number is also dimensionless
- Cr_max is typically constrained to be 2, i.e. in a given time step, one particle should not travel beyond the neighbouring element.
- Necessary condition when using explicit time integration scheme with the finite difference method.