

METRO MEtallurgical TRaining On-line



Spatial discretization techniques

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Education and Culture



Introduction



- Many physical phenomena are described by partial differential equations (PDEs).
- Analytical solutions are impossible to obtain except for linear equations on simple geometries.
- Since the computer memory is limited, discretization of the problem is necessary. Numerical methods can give *approximate* solutions of PDEs.
- Spatial discretization obtain the solution in a set of points rather that in the entire domain.





Simple one-dimensional Poisson equation

$$\frac{d^2 u}{dx^2} = 2, \quad 0 < x < 1$$

with Dirichlet boundary conditions

$$u(a) = u(0) = 0, \quad u(b) = u(1) = 0$$

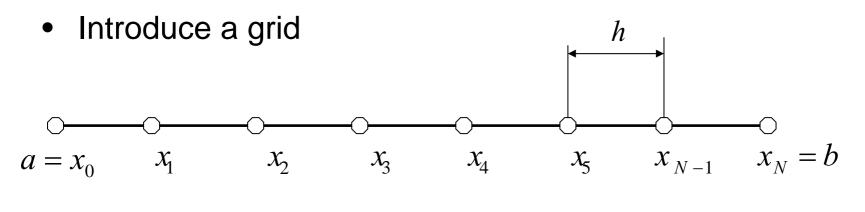
will be solved numerically using

- the finite difference method (FDM),
- the finite element method (FEM),
- the finite volume method (FVM).



Solution of a simple problem using the finite difference method





$$h_i = x_{i+1} - x_i = h, \quad i = 0, 1, \dots N - 1$$

- Approximate the differential equation at each grid point
- Solve the resulting system of algebraic equations





- By definition the derivative $\frac{du}{dx} = \lim_{h \to 0} \frac{u(x+h) u(x)}{h}$
- Finite difference approximation at point x_i

$$\left(\frac{du}{dx}\right)_{i} \approx \frac{u\left(x_{i}+h\right)-u\left(x_{i}\right)}{h} = \frac{u_{i+1}-u_{i}}{h} \quad \text{forward difference}$$

$$\left(\frac{du}{dx}\right)_{i} \approx \frac{u_{i}-u_{i-1}}{h} \quad \left(\frac{du}{dx}\right)_{i} \approx \frac{u_{i+1}-u_{i-1}}{2h}$$

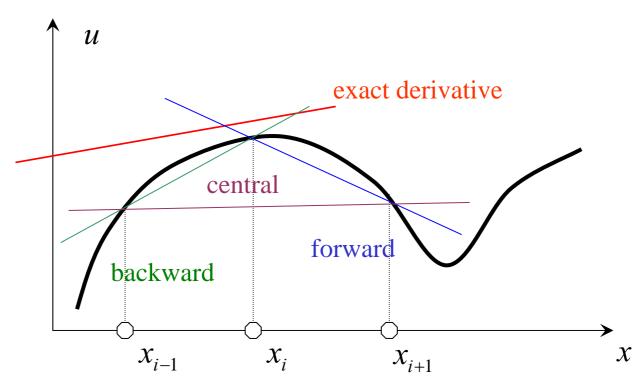
backward difference

central difference





• Forward, backward and central differences



• Central difference is the most accurate

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• Approximation of second derivative

$$\frac{d^2 u}{dx^2} = \frac{d}{dx} \left(\frac{du}{dx}\right) \approx \frac{(du / dx)(x+h) - (du / dx)(x)}{h}$$

• Use central differences for du / dx

$$\frac{d^{2}u}{dx^{2}} \approx \frac{1}{h} \left[\frac{u_{i+1} - u_{i}}{h} - \frac{u_{i} - u_{i-1}}{h} \right] = \frac{u_{i-1} - 2u_{i} + u_{i+1}}{h^{2}}$$





• In our problem assume three grid points

$$x_0 = 0, \quad x_1 = 0.5, \quad x_2 = 1, \quad h = 0.5$$

• Difference equation for the point x_1

$$\frac{u_0 - 2u_1 + u_2}{h^2} = 2 \qquad \text{or} \qquad \frac{0 - 2u_1 + 0}{0.5^2} = 2$$

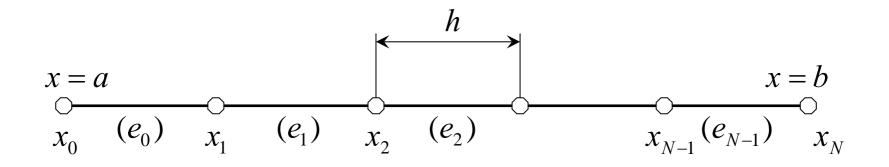
- One equation is needed for one unknown
- The solution is $u_1 = -0.25$



Solution of a simple problem using the finite element method



Subdivide the domain into finite elements (e.g. line segments in 1D, triangles or quadrilaterals in 2D, tetrahedra in 3D)







 Assume approximating function in each element, e.g. a linear polynomial

$$u_{h}^{(0)}(x) = \alpha_{1} + \alpha_{2}x$$
 for the element 0

• Parameters α_j can be determined easily

$$u_{h}^{(0)}(0) = \alpha_{1} + \alpha_{2}0 = u_{0}$$

$$u_{h}^{(0)}(h) = \alpha_{1} + \alpha_{2}h = u_{1} \text{ , hence } \alpha_{1} = u_{0}, \ \alpha_{2} = \frac{u_{1} - u_{0}}{h}$$

• Substituting yields

$$u_{h}^{(0)}(x) = \left(1 - \frac{x}{h}\right)u_{0} + \frac{x}{h}u_{1} = N_{0}(x)u_{0} + N_{1}(x)u_{1}$$

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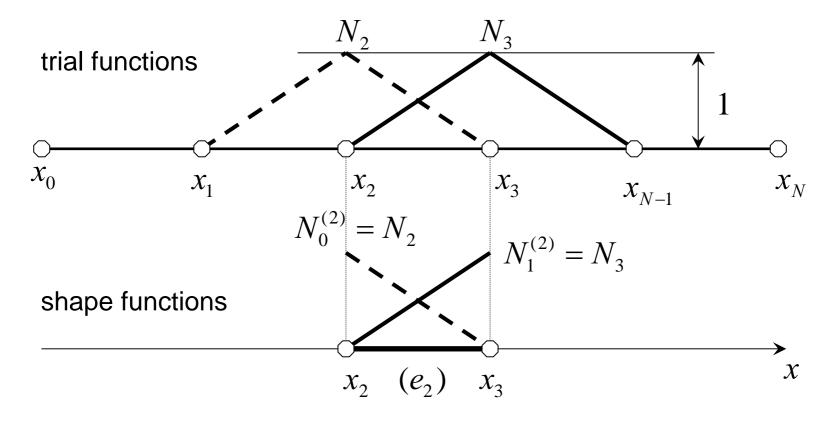
The function $N_{i}(x)$ is a *trial* function. It has the property

$$N_{j}(x) = \begin{cases} 1 & \text{at } x_{j} \\ 0 & \text{elsewhere Then } u_{h}(x) = \sum_{j=0}^{N} N_{j}(x)u_{j} \end{cases}$$
$$\frac{N_{2}}{\sqrt{N_{3}}} = \frac{N_{2}}{\sqrt{N_{3}}} = \frac{N_{2}}{\sqrt{N_{3}}$$





Trial function is called *shape* function when restricted to a finite element







Obtain an integral form of the problem, for example using the *weighted residual method*

Make the residual
$$R(x) = \frac{d^2 u_h}{dx^2} - 2$$
 "vanish", e.g.

 $\int_{\Omega} W(x)R(x)d\Omega = 0, \quad W(x) \text{ is a test or weighting function}$

W(x) = N(x) is a possible choice. Then

 $\left|\int_{\Omega} N_{i}(x)R(x)d\Omega = 0, \quad i = 0, 1, \dots, N\right|$

Galerkin finite element method





Assumed solution is piecewise linear and does not have second-order derivative. Integrate by parts

$$\int_{a}^{b} N_{i} \left(\frac{d^{2}u_{h}}{dx^{2}} - 2 \right) dx = \int_{a}^{b} \left(-\frac{dN_{i}}{dx} \frac{du_{h}}{dx} - 2N_{i} \right) dx + N_{i} \frac{du_{h}}{dx} \Big|_{a}^{b}$$

Now only the first derivative is necessary

$$\frac{du_{h}(b)}{dx} \cdot 1 \quad \text{and} \quad \frac{du_{h}(a)}{dx} \cdot (-1) \quad \text{are normal fluxes } q_{n}$$

imposed in Neumann boudary conditions





• The weak form of the problem reads

$$\int_{a}^{b} \frac{dN_{i}}{dx} \frac{du_{h}}{dx} dx = \int_{a}^{b} (-2) N_{i} dx + N_{i} q_{n} (a) + N_{i} q_{n} (b)$$
$$i = 0, 1, \dots, N$$

• Derivative of the solution is also approximated

$$u_{h} = \sum_{j=0}^{N} N_{j} u_{j} \qquad \frac{du_{h}}{dx} = \sum_{j=0}^{N} \frac{dN_{j}}{dx} u_{j}$$





Substituting and shifting sum gives for i = 0, 1, ..., N

$$\sum_{j=0}^{N} \left(\int_{a}^{b} \frac{dN_{i}}{dx} \frac{dN_{j}}{dx} dx \right) u_{j} = \int_{a}^{b} (-2)N_{i}dx + N_{i}q_{n}(a) + N_{i}q_{n}(b)$$

which is a system of linear algebraic equations

$$\sum_{j=0}^{N} k_{ij} u_{j} = f_{i} + g_{i}, \quad i = 0, 1, ..., N \quad \text{or} \quad \mathbf{K} \mathbf{u} = \mathbf{f} + \mathbf{g}$$

- K stiffness matrix u unknown nodal values
- f source vector g flux vector





• Integrals can be evaluated by summing contributions from individual elements

$$\int_{\Omega} (\cdot) d\Omega = \sum_{elements} \int_{\Omega_e} (\cdot) d\Omega$$

• Integrals involving N_i are nonzero only in elements containing the node i, e.g.

$$\int_{\Omega} (-2) N_i d\Omega = \int_{\Omega_i} (-2) N_1^{(i)} d\Omega + \int_{\Omega_{i+1}} (-2) N_0^{(i+1)} d\Omega$$





This leads to a local system of equations for each element *e*

$$\mathbf{K}^{(e)}\mathbf{u}^{(e)} = \mathbf{f}^{(e)} + \mathbf{g}^{(e)}$$

$$k_{ij}^{(e)} = \int_{\Omega_e} \frac{dN_i^{(e)}}{dx} \frac{dN_j^{(e)}}{dx} dx, \quad i, j = 0,1$$

$$f_i^{(e)} = \int_{\Omega_e} (-2) N_i^{(e)} dx$$

 $g_i^{(e)} = N_i^{(e)} q_n$ (only in elements with Neumann boundary condition)





• The element integrals can be evaluated easily

$$\mathbf{K}^{(e)} = \frac{1}{h} \begin{bmatrix} 1 & -1 \\ -1 & 1 \end{bmatrix} \qquad \qquad \mathbf{f}^{(e)} = -h \begin{bmatrix} 1 \\ 1 \end{bmatrix}$$

 Assuming the mesh with 3 nodes and 2 elements, the local systems are

$$\frac{1}{h} \begin{bmatrix} 1 & -1 \\ -1 & 1 \end{bmatrix} \begin{cases} u_0^{(0)} \\ u_1^{(0)} \end{cases} = -h \begin{bmatrix} 1 \\ 1 \end{bmatrix}, \quad \frac{1}{h} \begin{bmatrix} 1 & -1 \\ -1 & 1 \end{bmatrix} \begin{cases} u_0^{(1)} \\ u_1^{(1)} \end{cases} = -h \begin{bmatrix} 1 \\ 1 \end{bmatrix}$$





Using global indices and augmenting gives

$$\frac{1}{h} \begin{bmatrix} 1 & -1 & 0 \\ -1 & 1 & 0 \\ 0 & 0 & 0 \end{bmatrix} \begin{bmatrix} u_0 \\ u_1 \\ u_2 \end{bmatrix} = -h \begin{bmatrix} 1 \\ 1 \\ 0 \end{bmatrix} \quad \text{for element (0)}$$

$$\frac{1}{h} \begin{bmatrix} 0 & 0 & 0 \\ 0 & 1 & -1 \\ 0 & -1 & 1 \end{bmatrix} \begin{bmatrix} u_0 \\ u_1 \\ u_2 \end{bmatrix} = -h \begin{bmatrix} 0 \\ 1 \\ 1 \end{bmatrix} \text{ for element (1)}$$





• Assemble the global system by summing up local systems

$$\frac{1}{h} \begin{bmatrix} 1 & -1 & 0 \\ -1 & 1+1 & -1 \\ 0 & -1 & 1 \end{bmatrix} \begin{bmatrix} u_0 \\ u_1 \\ u_2 \end{bmatrix} = -h \begin{bmatrix} 1 \\ 1+1 \\ 1 \end{bmatrix}$$

• Local contributions are overlapped (superimposed)





- In our example $u_0 = u_2 = 0$
- Equation for the node 1

$$\frac{-u_0 + 2u_1 - u_2}{0.5} = -2 \cdot 0.5 \quad \text{hence} \quad u_1 = -0.25$$

• The solution is identical to that of FDM (for this simple problem and geometry)



Solution of a simple problem using the finite volume method



- Partial differential equations that we solve express conservation of a quantity (energy, mass,etc.)
- Conservation equations can be written in integral form, e.g. for the Poisson equation

$$\int_{0}^{1} \frac{d^{2}u}{dx^{2}} dx = \int_{0}^{1} 2dx$$

• Change the volume integral to a surface integral

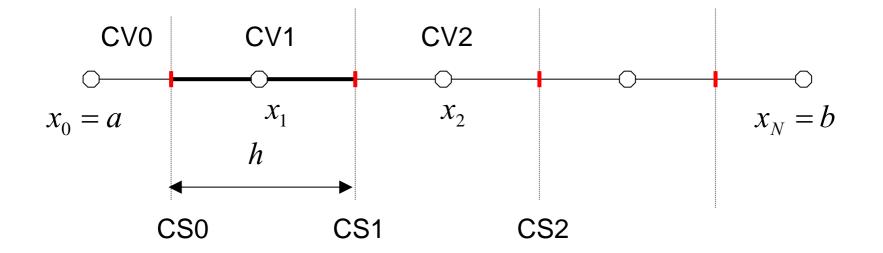
$$\frac{du}{dx}\Big|_{0}^{1} = \int_{0}^{1} 2dx$$

Balance: flux of a quantity entering and leaving the domain equals the amount produced internally by the source





The method utilises control volumes (finite volumes) and control surfaces



CV1 around node 1 has control surfaces CS0 and CS1. Control surfaces are located at line midpoints.





Balance equation is valid for each control volume

 $\frac{du}{dx}\Big|_{a}^{CS0} = \int_{CV0} 2dx \qquad \text{for control volume 0}$

$$\frac{du}{dx}\Big|_{CS\,0}^{CS\,1} = \int_{CV\,1} 2dx$$

for control volume 1

$$\frac{du}{dx}\Big|_{CS1}^{CS2} = \int_{CV2} 2dx$$

for control volume 2



- Flux is evaluated at control surfaces using e.g. finite differences
- By summing up equations for control volumes we obtain the global equation

$$\frac{du}{dx}\Big|_{a}^{CS_{0}} + \frac{du}{dx}\Big|_{CS_{0}}^{CS_{1}} + \frac{du}{dx}\Big|_{CS_{1}}^{CS_{2}} + \dots \frac{du}{dx}\Big|_{CS_{N-1}}^{b} = \frac{du}{dx}\Big|_{a}^{b}$$
$$\int (\cdot)dx + \int (\cdot)dx + \dots + \int (\cdot)dx = \int (\cdot)dx$$

(since fluxes through control surfaces cancel out)

 VC_N

Ω

 VC_0

 VC_1





• Flux is conserved between CV0 and CV1 through CS0 and between CV1 and CV2 through CS1 etc. provided approximation of du/dx is the same on both sides

Automatic conservation of a physical quantity is a distinct feature of FVM

• Flux at the control surface can be approximated in many ways, e.g.

$$\frac{du}{dx}\Big|_{x=CS_i} \approx \frac{u_{i+1} - u_i}{h}$$





• Assume three nodes and three control volumes for our problem. Balance equation for the volume 1 is

$$\frac{du}{dx}\Big|_{CS0}^{CS1} = \int_{CV1} 2dx \Longrightarrow \frac{du}{dx}\Big|_{x=CS1} - \frac{du}{dx}\Big|_{x=CS0} = \int_{CV1} 2dx$$

• Approximate derivatives with finite differences

$$\frac{u_2 - u_1}{h} - \frac{u_1 - u_0}{h} = 2h \Longrightarrow \frac{u_0 - 2u_1 + u_2}{h} = 2h$$

• The solution is the same as in FDM and FEM (for this simple problem and geometry)



Imposing the Neumann condition



Consider again the Poisson equation

$$\frac{d^2 u}{dx^2} = f(x) = 2, \quad 0 < x < 1$$

$$u(0) = u_0 = 0$$
 Dirichlet boundary condition

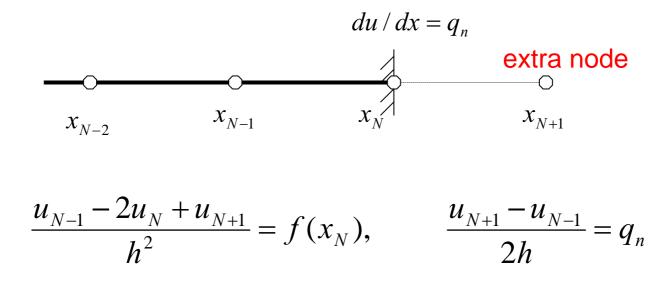
$$\frac{du}{dx}(1) = q_n = 1$$
 Neumann boundary condition



Imposing the Neumann condition in FDM



• One approach is to add a fictitious node on the right



• By eliminating u_{N+1} we obtain the equation for the node N

$$\frac{u_{N-1} - u_N}{h^2} = \frac{1}{2}f(x_N) - \frac{q_n}{h}$$

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Imposing the Neumann condition in FDM, cont.



- Us usual, assume 3 nodes in our problem
- Difference equation for the internal node 1

$$\frac{u_0 - 2u_1 + u_2}{h^2} = 2 \quad \text{or} \quad \frac{0 - 2u_1 + u_2}{0.5^2} = 2$$

• Equation for the node on the Neumann boundary

$$\frac{u_1 - u_2}{0.5^2} = \frac{2}{2} - \frac{1}{0.5}$$

• The solution is
$$u_1 = -0.25, u_2 = 0$$



Imposing the Neumann condition in FEM



- Neumann condition apears "naturally" in FEM equations as the result of integration by parts
- Since u_0 is known (Dirichlet b.c.) it can be eliminated from the system of equations
- In our two-element mesh only the last element (e₁) contributes to the flux vector g

$$\frac{1}{h} \begin{bmatrix} 2 & -1 \\ -1 & 1 \end{bmatrix} \begin{cases} u_1 \\ u_2 \end{cases} = -h \begin{bmatrix} 2 \\ 1 \end{bmatrix} + \begin{bmatrix} 0 \\ 1 \end{bmatrix}$$

$$N_2(b)q_n = 1 \cdot q_n = 1$$

• The solution is the same like in FDM (for this problem)



Imposing the Neumann condition in FVM



• Neumann data q_n appears explicitly in the balance equation for the boundary volume

$$\frac{du}{dx}\Big|_{CS_1}^b = \int_{CV2} 2dx \Longrightarrow q_n - \frac{du}{dx}\Big|_{x=CS1} = \int_{CV2} 2dx$$

• The system of equations is then

$$\frac{u_2 - u_1}{h} - \frac{u_1 - u_0}{h} = 2h, \qquad q_n - \frac{u_2 - u_1}{h} = 2\frac{h}{2}$$

• The solution is the same as in FDM and FEM (for this problem)



FDM, FEM and FVM for a 1D equation - conclusions



- FDM is the easiest to understand.
- Derivation of FEM equations is tedious.
- Only FVM has inherent conservative property.
- Neumann conditions are approximated in FDM, but appear directly in the formulation in FEM and FVM.
- All the methods gave identical solution. However, this happens only for simple problems and geometries.



Two-dimensional problems



 Γ_N

n

Consider the Poisson equation

$$-\frac{\partial}{\partial \mathbf{x}} \left(k \frac{\partial u}{\partial \mathbf{x}} \right) - \frac{\partial}{\partial \mathbf{y}} \left(k \frac{\partial u}{\partial \mathbf{y}} \right) = f(x, y) \text{ in } \Omega$$

with boundary conditions

$$u = u_D \quad \text{on } \Omega_D \quad \text{(Dirichlet)} \qquad \qquad \mathbf{1}_D \\ -k \frac{\partial u}{\partial n} = -k \left(\frac{\partial u}{\partial x} n_x + \frac{\partial u}{\partial y} n_y \right) = q_n \quad \text{on } \Omega_N \text{ (Neumann)}$$

For constant k

$$-k\left(\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2}\right) = f(x,y) \text{ in } \Omega$$

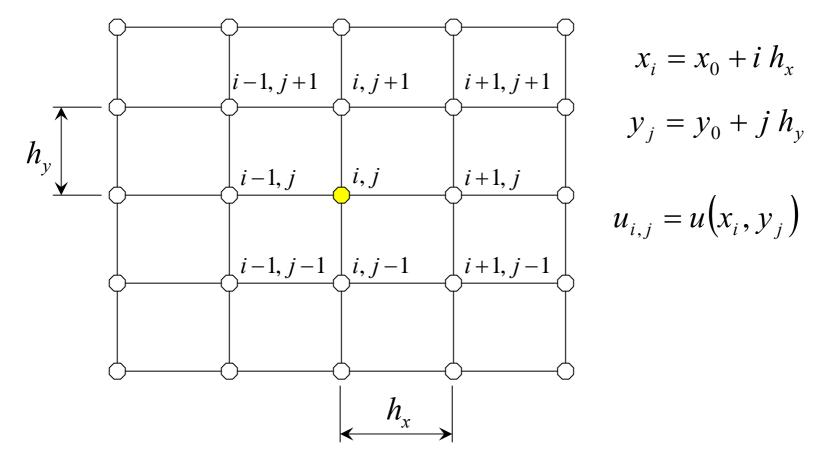
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The finite difference method in 2D



Each grid point has two indices







Finite difference formulas used for 1D problems can be used to approximate the partial derivatives at *i,j*, e.g.

$$\frac{\partial u}{\partial x} = \lim_{h \to 0} \frac{u(x+h, y) - u(x, y)}{h} \approx \frac{u_{i+1,j} - u_{i,j}}{h_x}$$

$$\frac{\partial u}{\partial y} = \lim_{h \to 0} \frac{u(x, y+h) - u(x, y)}{h} \approx \frac{u_{i,j+1} - u_{i,j}}{h_y}$$

(forward differences)





Approximation of partial derivatives

$$\left[\frac{\partial}{\partial \mathbf{x}}\left(k\frac{\partial u}{\partial \mathbf{x}}\right)\right]_{i,j} \approx \frac{\left(k\frac{\partial u}{\partial \mathbf{x}}\right)_{i+1/2,j} - \left(k\frac{\partial u}{\partial \mathbf{x}}\right)_{i-1/2,j}}{h_x}$$

(central difference)

$$\left[\frac{\partial}{\partial \mathbf{x}}\left(k\frac{\partial u}{\partial \mathbf{x}}\right)\right]_{i,j} \approx \frac{k_{i+1/2,j}\frac{u_{i+1,j}-u_{i,j}}{h_x}-k_{i-1/2,j}\frac{u_{i,j}-u_{i-1,j}}{h_x}}{h_x}$$
 (central difference of the second second

(central differences)

$$k_{i+1/2,j} = k \left(x_i + \frac{1}{2} h_x, y_j \right)$$

evaluated at the midpoint





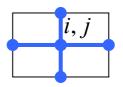
• Approximation of the Poisson equation at *i*,*j*

$$-\frac{k_{i+1/2,j}\frac{u_{i+1,j}-u_{i,j}}{h_x}-k_{i-1/2,j}\frac{u_{i,j}-u_{i-1,j}}{h_x}}{h_x}\cdots$$

$$-\frac{k_{i,j+1/2}\frac{u_{i,j+1}-u_{i,j}}{h_y}-k_{i,j-1/2}\frac{u_{i,j}-u_{i,j-1}}{h_y}}{h_y}=f_{i,j}$$

for each grid point except on the boundary

• Five unknowns per an equation





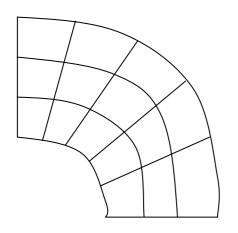


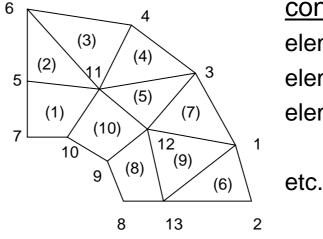
- FDM is the best suited for *structured* grids, where it is possible for the grid point *i,j* to
 - -compute its coordinates,
 - -determine its neighbours.
- In a structured grid all internal the nodes
 - -have the same number of neighbours,
 - -have the same number of cells around them.
- A grid point is located at intersection of two lines, each belonging to one of the two families of lines.
- The lines are not limited to horizontal/vertical.





Unstructured grids are more flexible but *connectivity* must be given explicitly







elem (1): 5 7 10 11

- elem (2): 11 6 5
- elem (3): 4 6 11

structured grid

(can compute indices of element nodes)

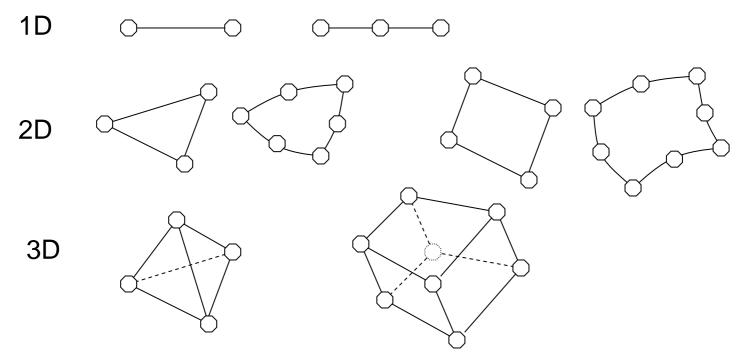
unstructured grid

(no pattern in numbering)





- Finite element method shows its advantages on unstructured grids and complex geometries
- A great variety of shapes can be used







- Derivation of the weak problem and finite element equations is similiar to that for 1D
- The weak form

$$\int_{\Omega} k \left(\frac{\partial N_i}{\partial x} \frac{\partial u}{\partial x} + \frac{\partial N_i}{\partial y} \frac{\partial u}{\partial y} \right) d\Omega = \int_{\Omega} N_i f d\Omega - \int_{\Gamma} N_i q_n ds, \quad i = 0, 1, \dots, N$$

• Approximate solution in a triangular element (e) in terms of shape functions and nodal values

$$u_h^{(e)} = \sum_{j=0}^2 N_j^{(e)}(x, y) u_j^{(e)} \qquad \qquad \frac{\partial u_h^{(e)}}{\partial x} = \sum_{j=0}^2 \frac{\partial N_j^{(e)}(x, y)}{\partial x} u_j^{(e)}$$





• Finite element equations for the element (e)

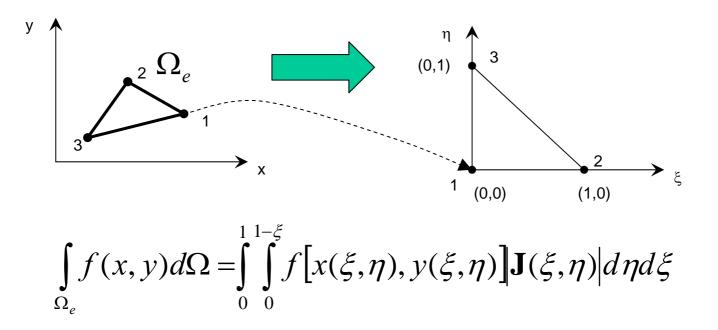
$$\int_{\Omega_{e}} k \left(\frac{\partial N_{i}^{(e)}}{\partial x} \frac{\partial N_{j}^{(e)}}{\partial x} + \frac{\partial N_{i}^{(e)}}{\partial y} \frac{\partial N_{j}^{(e)}}{\partial y} \right) d\Omega = \int_{\Omega_{e}} N_{i}^{(e)} f d\Omega - \int_{\Gamma_{N} \cap \partial \Omega_{e}} N_{i}^{(e)} q_{n} ds$$
$$i, j = 0, 1, 2$$

- It is a local system of equation. The size equals the number of nodes in the element (3 - triangle, 4 -quadrilateral, 6 - a second-order triangle)
- As usual, the global system of equations is assembled from such local systems





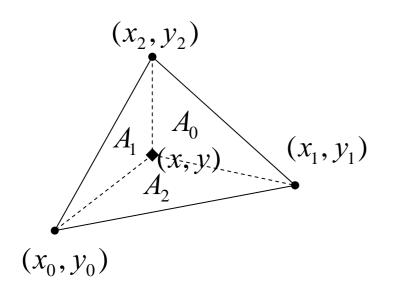
- Numerical integration is used for evaluation of volume and surface integrals
- It is much easier to integrate over regular triangles or squares. This involves *mapping*





Shape functions of the linear triangular element

• Area coordinates



$$L_0(x, y) = A_0 / A$$
$$L_1(x, y) = A_1 / A$$
$$L_2(x, y) = A_2 / A$$

A - element area

 $L_i = \begin{cases} 1 & \text{at the node} (x_i, y_i) \\ 0 & \text{at other nodes} \end{cases}$

• Shape functions are the area coordinates $N_i = L_i, i = 0,1,2$

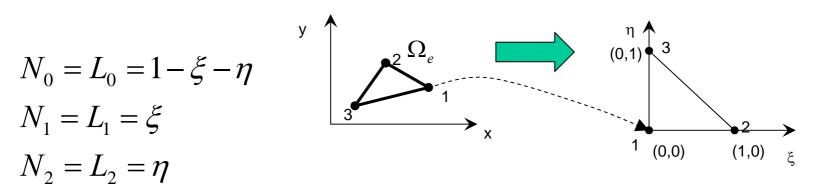






Coordinate mapping for the linear triangular element





$$x(\xi,\eta) = x_0 + (x_1 - x_0)\xi + (x_2 - x_0)\eta$$

$$y(\xi,\eta) = y_0 + (y_1 - y_0)\xi + (y_2 - y_0)\eta$$

$$|\mathbf{J}| = 2A$$
 $\frac{\partial N_i}{\partial x} = \text{const}, \ \frac{\partial N_i}{\partial y} = \text{const}$



The finite volume method in 2D



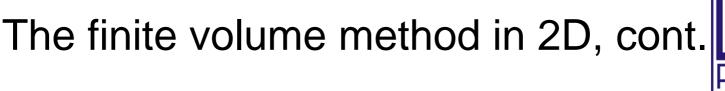
- Derivation of the balance equation is similiar to that for 1D
- Invoking the divergence theorem

$$\int_{\Omega} \left[\frac{\partial}{\partial x} \left(k \frac{\partial u}{\partial x} \right) + \frac{\partial}{\partial y} \left(k \frac{\partial u}{\partial y} \right) \right] d\Omega = \int_{\Gamma} k \left(\frac{\partial u}{\partial x} n_x + \frac{\partial u}{\partial x} n_y \right) ds = \int_{\Gamma} (-q_n) ds$$

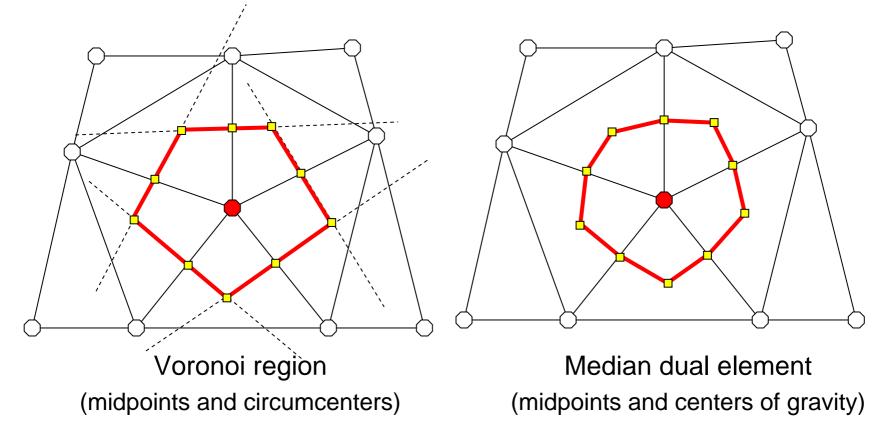
• Integral conservation equation for the Poisson equation is simply

$$\int_{\Gamma} q_n ds = \int_{\Omega} f d\Omega$$

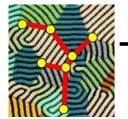


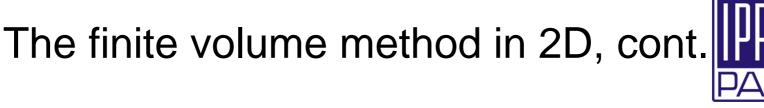


Dual mesh is the mesh of finite volumes around nodes of a mesh of triangles or quadrilaterals

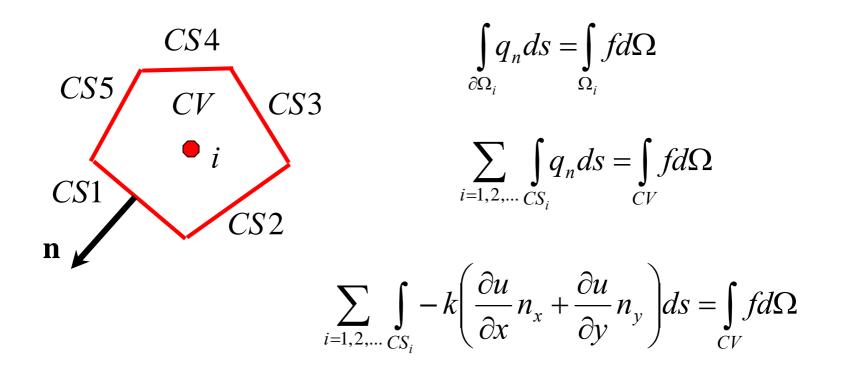


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Balance equation for a finite volume around node *i*







• Integrals are evaluated numerically.

$$\int_{CV} f d\Omega \approx f(x_i, y_i) \cdot \text{Volume}(CS)$$

$$\int_{CS} q_n ds \approx q_n (\text{middle}) \cdot \text{Area}(CS)$$

- Interpolation of partial derivatives in the middle of the control surface
 – central finite differences
 - -using finite element shape functions