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FINITE ELEMENT METHOD ON 3D MESH WITH LAYER STRUCTURE – APPLICATION ON FLOW AND TRANSPORT IN POROUS MEDIA*

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Abstract

We introduce a formulation of the finite element method (FEM) adapted to typical geometry of groundwater problems. The three-dimensional domain is discretized in the following way: the projection to the horizontal plane is a triangulation (unstructured mesh) and the mesh is composed of layers in the space. Thus there is need to define finite elements on trilateral prims. We show an alternative numerical solution of porous media (potential) flow by means of combining the FEM on 2D triangle mesh and finite differences in the vertical direction (1D columns of mesh nodes). This approach correspond to the fact that the horizontal dimension is much larger then the vertical in the groundwater problems. The same numerical scheme can be also formulated in terms of finite volume method, providing the mass balance property, important for subsequent solution of the solute transport problem.

1. Introduction

The problems of groundwater flow and solute transport are well known as cases for numerical solution, with important application in mining technologies and environmental protection. The current trend is the use of finite element and finite volume method with increasing flexibility in problem geometry and input data. But it is mostly difficult to measure all the input values in the governing equations and it is often useful to adjust the model structure to the available input data. Such a case is a construction of numerical model based on 3D mesh of trilateral prisms with layered structure – based on the unstructured triangulation in horizontal projection and set of columns and layers in the vertical direction, which correspond to the structure of sedimented rock.

The trilateral prismatic shape is not the standard case for the finite element method. We cannot simply define the lowest order (linear) base function on this shape. The apparently possible approaches are the bilinear functions derived from the trilinear base function on hexahedron, or a decomposition of prism to three tetrahedra with linear base function. The problem can be also solved in certain sense more simply, starting from the definition of 2D finite element on triangles. The method also keeps the nice property of the linear finite elements concerning

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the mass balance resulting from the equivalence with finite volume method [2]. The proposed model is related to the standard approaches e.g. in the following ways:

- It is a generalization of finite differences on rectangular (quadrilateral) mesh in vertical plane.
- It is a generalisation of quasi-3D model, where horizontal geological objects are considered instead of numerical discretization: each groundwater collector is represented as 2D (horizontal) and the communication through isolators is added; see [4], [7].

2. Problem description

We consider the porous media fluid flow problem, i.e. fluid flow governed by the Darcy's law (see [1]). In the steady state, we solve the second-order elliptic equation

$$-\nabla \cdot (K \nabla h) = q \tag{1}$$

where h is the piezometric head $h = \frac{p}{\varrho g} + z$, K is the hydraulic conductivity (tensor), q is the rate of sources/sinks, p is the pressure, ϱ is the density, and g is the gravity acceleration. Besides h, there is the velocity $u = K\nabla h$ as the unknown of interest.

The problems are typically described by mixed boundary conditions, i.e. the boundary $\Gamma = \partial\Omega$ consist of parts $\overline{\Gamma}_1 \cup \overline{\Gamma}_2 \cup \overline{\Gamma}_3 = \overline{\partial\Omega}$, where:

- Dirichlet boundary condition $h = h_D$ is prescribed on Γ_1
- Neumann boundary condition $\nabla h \cdot \vec{\nu} = u_N$ is prescribed on Γ_2
- third type (Newton) boundary condition $\nabla h \cdot \vec{\nu} = \sigma(h - h_3)$ is prescribed on Γ_3

We will use this most simple problem for the derivation of the numerical method, which can be in the same way formulated for the more complex cases, like unsteady flow with saturated–unsaturated interface.

3. Discretization

The mesh topology is derived from a unstructured triangulation in 2D (horizontal projection of the 3D mesh): We consider a set of nodes in a vertical line associated with a node of 2D triangulation (we call it "multi-node"). The mesh consist of layers, each with the same triangulation, with vertically connected nodes. In the sense of volumetric objects, the mesh consists of trilateral prisms, ordered to columns ("multi-elements") and layers (Fig. 1). In general, the layers (i.e. bases of prisms) do not need to be horizontal. We also admit two degenerated objects arising from prism by merging one or two vertical pairs of nodes (necessary to represent incomplete layers).

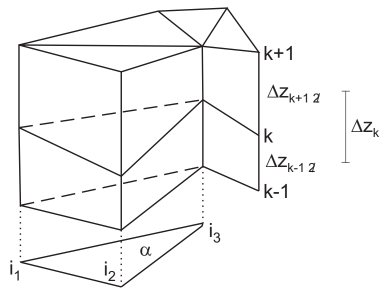

Fig. 1: *Structure of the layered mesh and notation of the position indexing.*

3.1. Notation of discrete quantities

We use indexing of objects by pair of "coordinates": horizontal position by index (or label) in unstructured triangulation and vertical position by index of layer (sequential order). The nodes in horizontal projection (multi-nodes) are indexed with $i \in \{1, \dots, n_i\}$, where n_i is the total number of multi-nodes; we denote the projection coordinates x_i, y_i. The triangles in the horizontal projection (multi-elements) are denoted e_α, $\alpha \in \{1, \dots, n_\alpha\}$, where n_α is the total number of triangles, defined as triples of vertices (multi-nodes) $V(\alpha) = \{i_1, i_2, i_3\}$. We distinguish the planar layers (2D planes with triangulation) and volume layers (set of prisms between two adjacent planar layers). The planar layers are denoted as Ω_k, indexed by $k \in \{0, \dots, n_k\}$, with node vertical coordinates $z_{i,k}$. The volume layers indexing is determined by usual notation for 1D discretization with half-integers, i.e. $(k - \frac{1}{2})$ for $k \in \{1, \dots, n_k\}$. Thus the 3D discretization objects (i.e. elements for use by FEM) are indexed $e_{\alpha,k-\frac{1}{2}}$. The length of vertical edge (distance of nodes) is $\Delta z_{i,k-\frac{1}{2}} = z_{i,k} - z_{i,k-1}$ and we denote the "distance of elements" (and the vertical dimension of dual volume associated with node i, k) $\Delta z_{i,k} = \frac{1}{2}(\Delta z_{i,k-\frac{1}{2}} + \Delta z_{i,k+\frac{1}{2}})$. See figure 1.

We also mention the notation for model input data according to above rules. We consider the hydraulic conductivity in the form

$$K = diag(K^{xy}, K_z) \quad \text{where } K^{xy} = \begin{pmatrix} K_x & K_{xy} \\ K_{xy} & K_y \end{pmatrix}$$

considering K^{xy} positive definite and $K_z > 0$. This is a special case of general conductivity tensor, which is symmetric positive definite following the physical principles. We denote the conductivity values associated with 3D element as $K^{xy}_{\alpha,k-\frac{1}{2}}$ and $K^{z}_{\alpha,k-\frac{1}{2}}$ (i.e. the piece-wise constant inhomogeneity). The sources/sinks will be used as associated with either elements $(Q_{\alpha,k-\frac{1}{2}})$ or nodes (dual volumes) $Q_{i,k}$.

We denote the unknown values of the piezometric head in the following way to distinguish the semi-discrete and fully discrete case: the discretization in the z-direction is set of functions in R^2 for all layers, i.e. $h_k(x, y)$ and the node values (fully discretized) are $H_{i,k}$.

3.2. Dual mesh

We understand the term dual mesh in general as mesh of volumes associated with nodes of the original mesh, with interfaces associated with edges of the original (primal) mesh. For exact definitions under various assumptions we refer to [2]. We use the dual mesh to derive the conservative approximation of velocity in section 4.4. (necessary for subsequent solute transport calculation). The notation used for indexing the unknown variables is simply the same as for nodes, i.e. i for unstructured horizontal position and k for vertical order. We note that the primal mesh variables are indexed with α for triangle and $(k-\frac{1}{2})$ for layer.

4. Numerical scheme

4.1. Discretization of the problem in 2D×1D structure

We consider the equation of porous media flow (1). We separate the derivatives in xy direction (horizontal) and in the z direction (vertical). With the assumption $K_{xz} = K_{yz} = 0$ and using the above notation for remaining components of K, we obtain

$$-\nabla_{xy} \cdot (K_{xy} \nabla_{xy} h) - \frac{\partial}{\partial z}\left(K_z \frac{\partial h}{\partial z}\right) = q \qquad \nabla_{xy} = \left(\frac{\partial}{\partial x}, \frac{\partial}{\partial y}\right) \tag{2}$$

We discretize the z derivatives with first-order differences and apply the standard transformation of the first term leading to the weak formulation. We consider a particular surface layer Ω_k and the Sobolev space $H^1(\Omega_k)$. Omitting the boundary conditions, we derive

$$(K^{xy} \nabla_{xy} h_k, \nabla_{xy} \phi_k)_{\Omega_k} - \left(\frac{1}{\Delta z_k}\left[K^z_{k+\frac{1}{2}} \frac{h_{k+1} - h_k}{\Delta z_{k+\frac{1}{2}}} - K^z_{k-\frac{1}{2}} \frac{h_k - h_{k-1}}{\Delta z_{k-\frac{1}{2}}}\right], \phi_k\right)_{\Omega_k} =$$
$$= (q_k, \phi_k)_{\Omega_k} \tag{3}$$

which must hold for all k (layers). We note that the semi-discrete values h_k and $K^z_{k+\frac{1}{2}}$ are only associated with layer, not with element or node.

We use the standard piece-wise linear finite-element approximation, i.e. the unknown function h_k (for a particular layer) is expressed as

$$h_k(x,y) = \sum_{j=1}^{n_i} H_{j,k} \phi_j^k(x,y), \qquad \phi_j^k(x_i, y_i) = \delta_{ij} \quad \text{pcw. linear} \tag{4}$$

where we introduced the node values $H_{j,k}$ (here the subscript j represent the meaning of i, i.e. mesh projection node). We also apply the “mass lumping” technique for the second term in (3), in similar way as the time-dependent problems [5]. The resulting finite-element/finite-difference scheme is

$$\Delta z_k \sum_{j=1}^{n_i} A^k_{ij} H_{j,k} - a H_{i,k+1} + b H_{i,k} - a H_{i,k-1} = \sum_{\alpha, i \in V(\alpha)} Q_{\alpha,k} \frac{S_\alpha}{3} \Delta z_k \qquad \forall i, k \tag{5}$$

where

$$a = \sum_{\alpha, i \in V(\alpha)} \frac{K^z_{\alpha,k+\frac{1}{2}} \frac{S_\alpha}{3}}{\Delta z_{i,k+\frac{1}{2}}}, \ b = a + c, \ c = \sum_{\alpha, i \in V(\alpha)} \frac{K^z_{\alpha,k-\frac{1}{2}} \frac{S_\alpha}{3}}{\Delta z_{i,k-\frac{1}{2}}}$$

and the 2D layer FE stiffness matrix is $A^k_{ij} = (K^{xy} \nabla_{xy} \phi^k_i, \nabla_{xy} \phi^k_j)_{\Omega_k}$.

4.2. Local matrix formulation

The scheme (5) can be regarded as a finite element method with unspecified base function on trilateral prism. Any set of base function with variables in nodes produce a local matrix 6×6. As well the scheme (5) can be written by assembly of "prism local matrices" in the form

$$\mathbb{A}^{(\alpha,k-\frac{1}{2})} = \frac{\Delta z_{i,k-\frac{1}{2}}}{2} \begin{pmatrix} \mathbb{A}^{(\alpha,k-1)} & 0 \\ 0 & \mathbb{A}^{(\alpha,k)} \end{pmatrix} + \frac{1}{3} \begin{pmatrix} \tau(i_1) & 0 & 0 & -\tau(i_1) & 0 & 0 \\ 0 & \tau(i_2) & 0 & 0 & -\tau(i_2) & 0 \\ 0 & 0 & \tau(i_3) & 0 & 0 & -\tau(i_3) \\ -\tau(i_1) & 0 & 0 & \tau(i_1) & 0 & 0 \\ 0 & -\tau(i_2) & 0 & 0 & \tau(i_2) & 0 \\ 0 & 0 & -\tau(i_3) & 0 & 0 & \tau(i_3) \end{pmatrix} \tag{6}$$

where $(\alpha, k-\frac{1}{2})$ is determination of the respective prismatic element, $\tau(i) = \dfrac{K^z_{\alpha,k-\frac{1}{2}} S_\alpha}{\Delta z_i}$ and i denote the nodes of the triangle in the horizontal projection $V(\alpha) = \{i_1, i_2, i_3\}$. The first term is block diagonal matrix composed of local matrices of 2D finite elements on triangle (upper/lower base of prism), i.e. $[\mathbb{A}^{(\alpha,k)}]_{i,j} = (\phi^k_i, \phi^k_j)_{e_{(\alpha,k)}}$ (scalar product of base functions (4)). The second term represents the finite difference method in vertical direction.

4.3. Physical formulation of the scheme

We can also derive the scheme (5) by different way, which is physically illustrative and allows the non-horizontal layers in contrast with the approach with separation of z and xy cartesian coordinates. We consider a FE scheme of 2D flow in a layer (normalised to a thickness $\Delta z_{i,k}$), where the communication with neighbouring layers is represented by source/sink, i.e.

$$\Delta z_{i,k} \sum_{j=1}^{n_i} A^k_{ij} H_{j,k} = (q_k, \phi_k)_{\Omega_k} + (\tilde{q}_k, \phi_k)_{\Omega_k} \tag{7}$$

where the term $\tilde{q}_k$ is the total flux for two neighbour layers:

$$\tilde{q}_{i,k} = \frac{[K^z S_i]_+}{\Delta z_{i,k+\frac{1}{2}}} (H_{i,k+1} - H_{i,k}) + \frac{[K^z S_i]_-}{\Delta z_{i,k-\frac{1}{2}}} (H_{i,k-1} - H_{i,k}) \tag{8}$$

and $[K^z S_i]_\pm = \sum_{\alpha, i \in V(\alpha)} K^z_{\alpha,k\pm\frac{1}{2}} \frac{S_\alpha}{3}$. This scheme is in fact formulated for the dual mesh: the thickness of the layer is $\Delta z_{i,k}$ and the cross-section area of a "channel" along the primal mesh edge is $\sum_{\alpha, i \in V(\alpha)} \frac{S_\alpha}{3}$ (in the scheme weighted with K_z).

4.4. Approximation of velocity

The approximation of velocity by means of fluxes along edges follows from the equivalence between the piecewise-linear finite-element method and cell-centred finite volume method on dual mesh. This approach is referred as control-volume FEM [2], [3]. The FV transmissibilities are equal to FE stiffness matrix components, allowing to express the fluxes between nodes ("dual" control volumes) as simply for node pressure results of FEM as for FV formulation.

We can directly apply all these properties in a particular layer (2D linear FEM), i.e. the fluxes between nodes i and j are $u_{ij} = A_{ij}(H_i - H_j)$ (up to normalisation with layer thickness). The vertical flux was expressed by the equation (8). Comparing the terms in (8) with the component of local and global stiffness matrices of the finite-element/finite-difference scheme (5), we derive that for both cases (horizontal and vertical edge) the corresponding off-diagonal matrix component can be used as transmissibility for flux calculation in the form $u_{IJ} = A_{IJ}(H_I - H_J)$ (here I and J represent the full index of node, i.e. $I = (i, k)$, A is the global stiffness matrix).

5. Conclusion

The presented numerical scheme for groundwater flow is implemented in the form of computer model with full interface for mesh, material parameters, and initial/boundary condition and successfully used for solution of large-scale hydrogeological problems in DIAMO Stráž pod Ralskem (see [6]). The model solves wider set of physical problem: unsteady water flow with unsaturated zone, advective transport, and density driven flow. We plan to publish the methods and results in another paper as well as a comparison with other finite-element approximations on prism, both in local matrix components and in results, to confirm the consistency.

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