Numerical Simulation of Transport Processes in Porous Media

Finite-Volume Methods

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November 3, 2009

Cell-Centred Finite-Volume Method

We want to discretise the steady-state ground-water equation

$$\nabla \cdot \vec{J}_w(\vec{x}) + r_w(\vec{x}) = 0$$

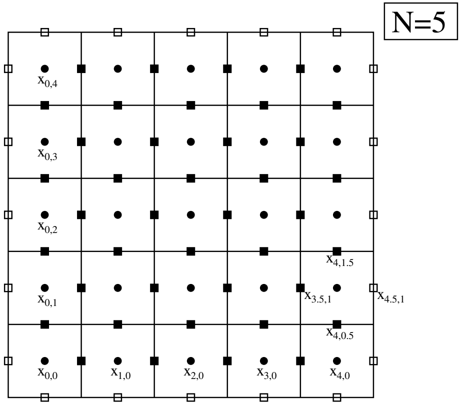
with

$$J_w = -K_s(\vec{x})\nabla p_w$$

with the Cell-Centred Finite-Volume method.

Divide Domain into Grid Cells

First we divide grid into rectangular grid cells g_{ij}



Transformation of Volume Integral into Boundary Integral

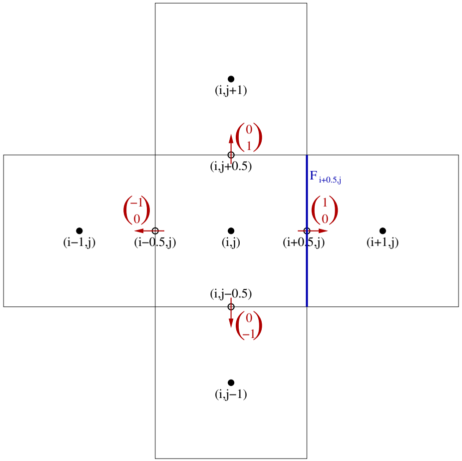
We demand that the integral of the partial differential equation over each grid cell is fulfilled:

$$\int\limits_{g_{ij}} \nabla \cdot \vec{J}_w \;\; dx\, dy = \int\limits_{g_{ij}} r(\vec{x}) \;\; dx\, dy$$

and use the Satz of Gauss to transform the volume integral over the divergence of the flux into a boundary integral over the flux normal to the boundary:

$$\underbrace{\Leftrightarrow}_{Satz\ of\ Gauss} \int\limits_{\partial g_{ij}} \vec{J}_w \cdot \vec{n} \;\; ds = \int\limits_{g_{ij}} r(\vec{x}) \;\; dx\, dy$$

Inner Grid Cell



Finite Volume Discretisation: Split into Sum over Faces

For our rectangular cell, we can split the integral over the boundary of the cell into integrals over each face

$$\int_{\partial g_{ij}} \vec{J}_w \cdot \vec{n} \; ds = \sum_{k=i\pm 0.5} \int_{F_{kj}} \vec{J}_w \cdot \vec{n} \; ds + \sum_{l=j\pm 0.5} \int_{F_{il}} \vec{J}_w \cdot \vec{n} \; ds$$

and approximate the integral over each face with the Midpoint rule

$$\underbrace{\approx}_{\text{Midpointrule}} \sum_{k=i\pm 0.5} \vec{J}_w(\vec{x}_{k,j}) \cdot \vec{n} \cdot \underbrace{h}_{\text{Face Area}} + \sum_{l=j\pm 0.5} \vec{J}_w(\vec{x}_{i,l}) \cdot \vec{n} \cdot \underbrace{h}_{\text{Face Area}}$$

If the permeability is a diagonal matrix the flux over a face depends only on the gradient in the normal direction

$$\vec{J}_w(\vec{x}) = -\begin{pmatrix} K_{xx}(\vec{x}) & 0 \\ 0 & K_{yy}(\vec{x}) \end{pmatrix} \cdot \begin{pmatrix} \frac{\partial p}{\partial x}(\vec{x}) \\ \frac{\partial p}{\partial y}(\vec{x}) \end{pmatrix}$$

Finite Volume Discretisation: Insert Flux law

The multiplication with the (normalised) normal vector only influences the sign of the flux integral

$$\sum_{k=i\pm 0.5} \vec{J}_w(\vec{x}_{k,j}) \cdot \vec{n} \cdot h + \sum_{l=j\pm 0.5} \vec{J}_w(\vec{x}_{i,l}) \cdot \vec{n} \cdot h =$$

$$-K_{xx}(\vec{x}_{i-0.5,j}) \cdot \frac{\partial p}{\partial x}(\vec{x}_{i-0.5,j}) \cdot \underbrace{(-1)}_{\text{from } n_x} \cdot h$$

$$-K_{xx}(\vec{x}_{i+0.5,j}) \cdot \frac{\partial p}{\partial x}(\vec{x}_{i+0.5,j}) \cdot \underbrace{(1)}_{\text{from } n_x} \cdot h$$

$$-K_{yy}(\vec{x}_{i,j-0.5}) \cdot \frac{\partial p}{\partial x}(\vec{x}_{i,j-0.5}) \cdot \underbrace{(-1)}_{\text{from } n_y} \cdot h$$

$$-K_{yy}(\vec{x}_{i,j+0.5}) \cdot \frac{\partial p}{\partial x}(\vec{x}_{i,j+0.5}) \cdot \underbrace{(1)}_{\text{from } n_y} \cdot h$$

Finite Volume Discretisation: Approximate Derivatives

The gradient at the face midpoint is approximated by a central difference quotient

$$\underbrace{\approx}_{\text{approx.Derivative}} \quad +K_{xx}(\vec{x}_{i-0.5,j}) \cdot \frac{p(\vec{x}_{i,j}) - p(\vec{x}_{i-1,j})}{h} \cdot h$$

$$-K_{xx}(\vec{x}_{i+0.5,j}) \cdot \frac{p(\vec{x}_{i+1,j}) - p(\vec{x}_{i,j})}{h} \cdot h$$

$$+K_{yy}(\vec{x}_{i,j-0.5}) \cdot \frac{p(\vec{x}_{i,j}) - p(\vec{x}_{i,j-1})}{h} \cdot h$$

$$-K_{yy}(\vec{x}_{i,j+0.5}) \cdot \frac{p(\vec{x}_{i,j+1}) - p(\vec{x}_{i,j})}{h} \cdot h$$

Finite Volume Discretisation: Approximate Derivatives

The integration of the source/sink term is also done with the midpoint rule:

$$\int_{g_{ij}} r(\vec{x})dx\,dy \approx h^2 r(\vec{x}_{i,j})$$

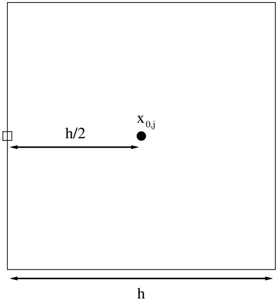
Matrix Contribution of each Grid Cell

We get one line of a linear equation system for each grid cell:

$$
\begin{aligned}
-K_{xx}(\vec{x}_{i-0.5,j}) \cdot p_{i-1,j} - K_{xx}(\vec{x}_{i+0.5,j}) \cdot p_{i+1,j} & \\
-K_{yy}(\vec{x}_{i,j-0.5}) \cdot p_{i,j-1} - K_{yy}(\vec{x}_{i,j+0.5}) \cdot p_{i,j+1} & \\
+\left[K_{xx}(\vec{x}_{i-0.5,j}) + K_{xx}(\vec{x}_{i+0.5,j}) + K_{yy}(\vec{x}_{i,j-0.5}) + K_{yy}(\vec{x}_{i,j+0.5})\right] \cdot p_{i,j} &= h^2 r(\vec{x}_{i,j})
\end{aligned}
$$

Dirichlet Boundary Conditions

Let us assume that at $x = 0$ there is a Dirichlet boundary:



The derivative between the face midpoint and the element midpoint can be approximated by a difference quotient (only first order):

$$\frac{\partial p}{\partial x}(\vec{x}_{-0.5,j}) \approx \frac{p(\vec{x}_{0,j}) - p_d(0, y_j)}{h/2}$$

Matrix Contribution at Dirichlet Boundary $x = 0$

The constant term $-K_{xx}(\vec{x}_{i-0.5,j}) \cdot p_d(0, y_j)$ is brought to the right-hand side of the equation:

$$\begin{aligned}
-K_{xx}(\vec{x}_{i+0.5,j}) \cdot p_{i+1,j} & \\
-K_{yy}(\vec{x}_{i,j-0.5}) \cdot p_{i,j-1} - K_{yy}(\vec{x}_{i,j+0.5}) \cdot p_{i,j+1} & \\
+ [2K_{xx}(\vec{x}_{i-0.5,j}) + K_{xx}(\vec{x}_{i+0.5,j}) & \\
+K_{yy}(\vec{x}_{i,j-0.5}) + K_{yy}(\vec{x}_{i,j+0.5})] \cdot p_{i,j} & = h^2 r(\vec{x}_{i,j}) + 2K_{xx}(\vec{x}_{i-0.5,j}) \cdot p_d(0, y_j)
\end{aligned}$$

Neumann Boundary Conditions

To integrate Neumann boundary conditions we go back to the point before the integration of the face fluxes with the midpoint rule. For each face we had to determine

$$\int_F \vec{J}_w \cdot \vec{n} \; ds$$

At a Neumann boundary $\vec{J}_w \cdot \vec{n}$ is given directly by the boundary condition $\phi_n(\vec{x})$, we can therefore use

$$\int_{F_{kl}} \vec{J}_w \cdot \vec{n} \; ds \underbrace{\approx}_{\text{Midpointrule}} h \cdot \vec{\phi}_N(\vec{x}) \cdot \vec{n}$$

at each Neumann boundary.

Matrix Contribution at Neumann Boundary $x = 0$

We transfer the constant term $h \cdot \phi_N(\vec{x}_{-0.5,j})$ to the right hand side:

$$\begin{aligned} -K_{xx}(\vec{x}_{i+0.5,j}) \cdot p_{i+1,j} & \\ -K_{yy}(\vec{x}_{i,j-0.5}) \cdot p_{i,j-1} - K_{yy}(\vec{x}_{i,j+0.5}) \cdot p_{i,j+1} & \\ +\left[K_{xx}(\vec{x}_{i+0.5,j}) + K_{yy}(\vec{x}_{i,j-0.5}) + K_{yy}(\vec{x}_{i,j+0.5})\right] \cdot p_{i,j} &= h^2 r(\vec{x}_{i,j}) - h \cdot \phi_N(\vec{x}_{-0.5,j}) \end{aligned}$$

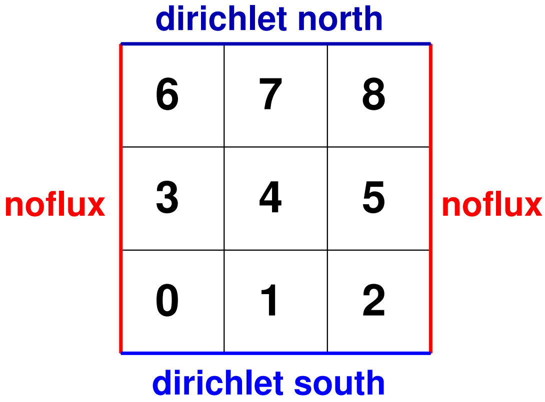
Different Grid Spacing in x and y direction

If the grid spacing in x and y direction is different, the h factors do not clear:

$$
\begin{aligned}
&-\frac{h_y}{h_x}\left(K_{xx}(\vec{x}_{i-0.5,j})\cdot p_{i-1,j} - K_{xx}(\vec{x}_{i+0.5,j})\cdot p_{i+1,j}\right)\\
&-\frac{h_x}{h_y}\left(K_{yy}(\vec{x}_{i,j-0.5})\cdot p_{i,j-1} - K_{yy}(\vec{x}_{i,j+0.5})\cdot p_{i,j+1}\right)\\
&\qquad\qquad\quad+\left[\frac{h_y}{h_x}\left(K_{xx}(\vec{x}_{i-0.5,j}) + K_{xx}(\vec{x}_{i+0.5,j})\right)\right.\\
&\qquad+\left.\frac{h_x}{h_y}\left(K_{yy}(\vec{x}_{i,j-0.5}) + K_{yy}(\vec{x}_{i,j+0.5})\right)\right]\cdot p_{i,j} \quad = \quad h_x h_y r(\vec{x}_{i,j})
\end{aligned}
$$

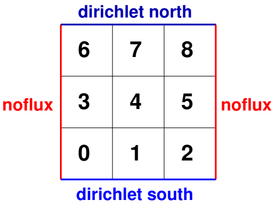
Example: 3×3 Grid

Let us perform a Finite-Volume discretisation of the stead-state groundwater equation on a 3×3 grid with a homogeneous permeability field and Dirichlet boundary condition on the north and south side and no-flux boundary conditions at the left and right:



$$K(\vec{x}) = \begin{pmatrix} K & 0 \\ 0 & K \end{pmatrix}$$

Example: 3×3 Grid



The resulting linear equation system is:

$$
\begin{pmatrix}
4K & -K & 0 & -K & 0 & 0 & 0 & 0 & 0 \\
-K & 5K & -K & 0 & -K & 0 & 0 & 0 & 0 \\
0 & -K & 4K & 0 & 0 & -K & 0 & 0 & 0 \\
-K & 0 & 0 & 3K & -K & 0 & -K & 0 & 0 \\
0 & -K & 0 & -K & 4K & -K & 0 & -K & 0 \\
0 & 0 & -K & 0 & -K & 3K & 0 & 0 & -K \\
0 & 0 & 0 & -K & 0 & 0 & 4K & -K & 0 \\
0 & 0 & 0 & 0 & -K & 0 & -K & 5K & -K \\
0 & 0 & 0 & 0 & 0 & -K & 0 & -K & 4K
\end{pmatrix}
\begin{pmatrix} p_0 \\ p_1 \\ p_2 \\ p_3 \\ p_4 \\ p_5 \\ p_6 \\ p_7 \\ p_8 \end{pmatrix}
=
\begin{pmatrix}
2Kp_{d_{\mathrm{south}}} \\ 2Kp_{d_{\mathrm{south}}} \\ 2Kp_{d_{\mathrm{south}}} \\ 0 \\ 0 \\ 0 \\ 2Kp_{d_{\mathrm{north}}} \\ 2Kp_{d_{\mathrm{north}}} \\ 2Kp_{d_{\mathrm{north}}}
\end{pmatrix}
$$

Effective Permeability

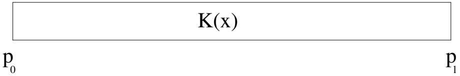
We assume that the permeability is a diagonal Tensor, which is depending on the position, but constant on each grid cell g_{ij}.
We need to evaluate K at the cell boundaries $x_{i\pm0.5,j\pm0.5}$.
What is the correct value of K if it is not homogeneous but element-wise constant?

1D-Example

The steady-state groundwater flow equation is:

$$\frac{dJ_w}{dx} = 0 \quad \text{in } \Omega = (0, \underbrace{\ell}_{\text{length}})$$

$$J_w = -K(x)\frac{dp}{dx}$$



with the Dirichlet boundary conditions

$$p(0) = p_0$$
$$p(\ell) = p_\ell$$

because of $\frac{dJ_w}{dx} = 0$ in $\Omega \Leftrightarrow J_w(x) = J_0 \in \mathbb{R}$ this means

$$J_0 = -K(x)\frac{dp}{dx} \Leftrightarrow \frac{dp}{dx} = -\frac{J_0}{K(x)}$$

1D-Example

By integration of both sides over the domain

$$\frac{dp}{dx} = -\frac{J_0}{K(x)}$$

$$\Leftrightarrow \int_0^\ell \frac{dp}{dx}dx = [p(x)]_0^\ell = p_\ell - p_0 = -J_0 \int_0^\ell \frac{1}{K(x)}dx$$

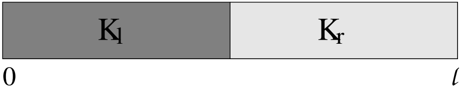
we get the flux depending on the boundary conditions and the permeability distribution:

$$\Leftrightarrow J_0 = - \underbrace{\frac{\ell}{\int_0^\ell \frac{1}{K(x)}dx}}_{\text{eff.permeability}} \cdot \underbrace{\frac{p_\ell - p_0}{\ell}}_{\text{approx.gradient}}$$

1D-Example, cell-wise constant Permeability

If we divide the domain into two halves with constant permeability

if $K(x) = \begin{cases} K_l & x \leq \frac{\ell}{2} \\ K_r & x > \frac{\ell}{2} \end{cases}$



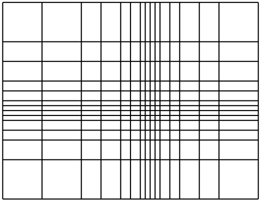
we can perform the integration and get the effective permeability

$$K_{\text{eff}} = \frac{\ell}{\int\limits_0^{\ell} \frac{1}{K(x)} dx} = \frac{\ell}{\frac{\ell}{2}\frac{1}{K_l} + \frac{\ell}{2}\frac{1}{K_r}} = \frac{2}{\frac{1}{K_l} + \frac{1}{K_r}}$$

We therefore choose for cell-wise constant permeabilities the harmonic mean

$$K(\vec{x}_{i\pm0.5,j}) = \frac{2}{\frac{1}{K(\vec{x}_{i,j})} + \frac{1}{K(\vec{x}_{i\pm1,j})}}$$

Finite-Volume Method for tensor-product Grids

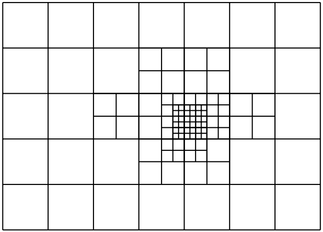


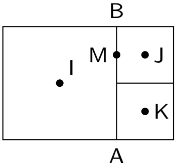
$$
\begin{aligned}
&-\frac{2h_{y_j}K_{xx}(\vec{x}_{i-0.5,j})}{h_{x_{i-1}}+h_{x_i}}\cdot p_{i-1,j}-\frac{2h_{y_j}K_{xx}(\vec{x}_{i+0.5,j})}{h_{x_i}+h_{x_{i+1}}}\cdot p_{i+1,j}\\
&-\frac{2h_{x_i}K_{yy}(\vec{x}_{i,j-0.5})}{h_{y_{j-1}}+h_{y_j}}\cdot p_{i,j-1}-\frac{2h_{x_i}K_{yy}(\vec{x}_{i,j+0.5})}{h_{y_j}+h_{y_{j+1}}}\cdot p_{i,j+1}\\
&+\left[\frac{2h_{y_j}K_{xx}(\vec{x}_{i-0.5,j})}{h_{x_{i-1}}+h_{x_i}}+\frac{2h_{y_j}K_{xx}(\vec{x}_{i+0.5,j})}{h_{x_i}+h_{x_{i+1}}}\right.\\
&\left.+\frac{2h_{x_i}K_{yy}(\vec{x}_{i,j-0.5})}{h_{y_{j-1}}+h_{y_j}}+\frac{2h_{x_i}K_{yy}(\vec{x}_{i,j+0.5})}{h_{y_j}+h_{y_{j+1}}}\right]\cdot p_{i,j} \quad = \quad h_{x_i}h_{y_j}r(\vec{x}_{i,j})
\end{aligned}
$$

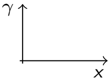
Complexer Grids with Cell-Centred Finite Volumes

With the Cell-Centred Finite Volume Method it is also possible to use some kind of unstructured grids:

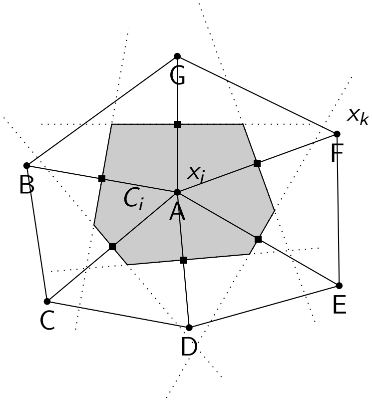
Nested Grids







Voronoi Grids



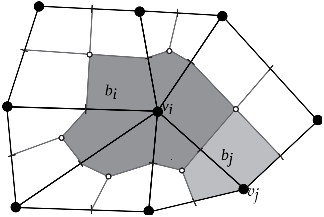
Summary Cell-Centred Finite-Volume Method

- Only the integral of the partial differential equation over each grid cell must fullfill the equation.
- Implementation of Dirichlet Boundary and Neumann Boundary conditions straight forward
- Structured and unstructured grids possible
- Dirichlet boundary conditions can easily be integrated by rearranging the equation systems and bringing them to the right side of the equation.
- Neumann boundary conditions can easily be integrated in the flux integrals
- Convergence order can differ dependent on the concrete method.

Properties of the Cell-Centred Finite-Volume Method

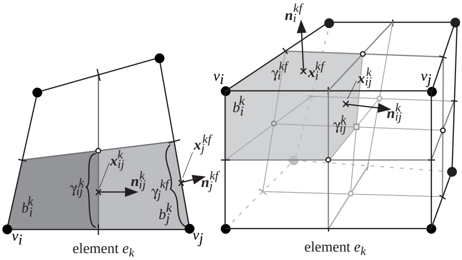
- Advantages:
  - well suited for structured grids
  - locally mass conservative
  - good approximation of average permeability
  - limited variety of unstructured grids possible
  - limited local adaptivity possible
  - cheap for simple problems
- Problems:
  - Only linear convergence rate on non-equidistant grids
  - grid generation can be complicated (must fulfil rather strong conditions)

The Vertex-Centred Finite-Volume Method



- The unknowns are located at the edges of the elements (vertices)
- Base functions are used on each element, which are parameterised with the values at the vertices
- A secondary mesh is constructed connecting the face centres and the barycenter of the element
- The flux balance is not calculated over the original grid, but over the secondary mesh, the elements of the secondary mesh are called control-volumes, the parts of a control volume belonging to a specific element of the primary mesh are called subcontrol-volumes.

The Vertex-Centred Finite-Volume Method (2)



- Material properties are assumed to be constant for each element
- The volume integrals are calculated as a sum over the subcontrol-volumes using the midpoint rule and the material properties valid for the specific control-volume. $\sum_i b_i^k \cdot r_i^k$
- The face integrals are calculated as a sum over all subcontrol-volume faces with the midpoint rule $\sum_{ij} \gamma_{ij}^k \vec{J}_{ij}^k \vec{n}_{ij}^k$
- The gradient at the face centres is given by the base functions.

Properties of the Vertex-Centred Finite-Volume Method

- Advantages:
  - can be used for domains with complicated shape
  - well suited for unstructured grids
  - local adaptivity possible
  - locally mass conservative
- Problems:
  - grid generation can be complicated (must often fullfill certain conditions)
  - more computationally expensive for simple problems
  - bad approximation of average permeability