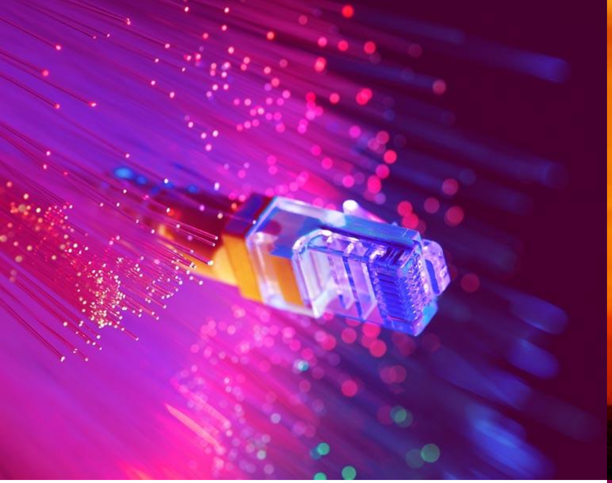

Elmer/Ice advanced workshop 2017

Grenoble, France


CSC – Finnish research, education, culture and public administration ICT knowledge center

How to write your own solver

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Outline

- We will discuss how to implement a simple Darcy flow problem
- We will discuss the derivation of the weak formulation from the PDE
- We will discuss the implementation of different (incl. natural) boundary conditions
- We will show how to modify the existing blueprint for advection-diffusion equations, Elmer's ModelPDE
- We will show how to compile the silver and how to include it in the SIF

Darcy flow

- Describes saturated flow in porous media
- Based on continuity of the groundwater flux, $\mathbf{J}_{gw}$:

$$\nabla \cdot \mathbf{J}_{gw} = S_{gw}$$

Where S_{gw} is the volumetric source of water

- The flux usually is given by

$$\mathbf{J}_{gw} = \mathbf{K}_{gw} \cdot (\rho_w \mathbf{g} - \nabla p)$$

Where $\mathbf{K}_{gw}$ is the (usually tensor-valued) hydraulic conductivity

NB: often the hydraulic head, including hydrostatic contribution is used instead – not so here

Weak formulation

- Applying weak formulation, i.e., integrating with test-function φ over whole domain Ω

$$\int_\Omega \nabla \cdot \mathbf{J}_{gw}\, \varphi\, dV = \int_\Omega S_{gw}\, \varphi\, dV$$

- Partial integration of l.h.s:

$$\int_\Omega \nabla \cdot \left(\mathbf{J}_{gw}\, \varphi\right)\, dV - \int_\Omega \mathbf{J}_{gw} \cdot \nabla \varphi\, dV = \int_\Omega S_{gw}\, \varphi\, dV$$

- Applying Green's [1)] theorem:

$$\oint_{\partial\Omega} \mathbf{J}_{gw} \cdot \mathbf{n}\, \varphi\, dV - \int_\Omega \mathbf{J}_{gw} \cdot \nabla \varphi\, dV = \int_\Omega S_{gw}\, \varphi\, dV$$

[1)] Gauss, for the German speakers

Weak formulation

- Inserting and rearranging for the unknown, the pressure:

$$\int_\Omega (\mathbf{K}_{gw} \cdot \nabla p) \cdot \nabla \varphi \, dV = \int_\Omega (\mathbf{K}_{gw} \cdot \mathbf{g} \rho_w) \cdot \nabla \varphi \, dV + \int_\Omega S_{gw} \, \varphi \, dV - \oint_{\partial\Omega} \mathbf{J}_{gw} \cdot \mathbf{n} \, \varphi \, dV$$

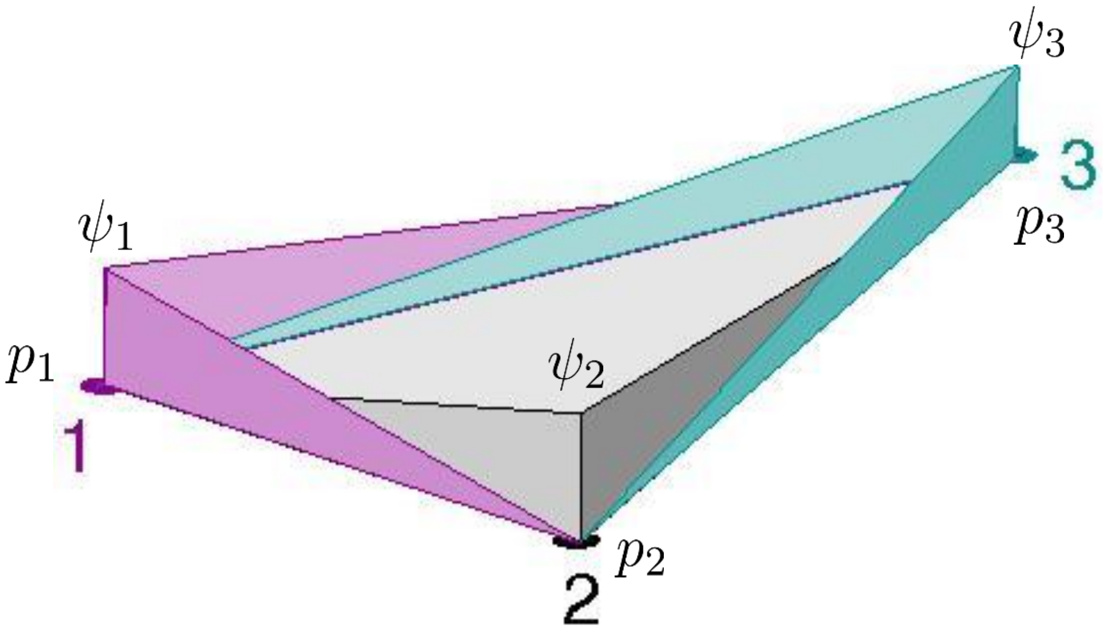
Left hand side

Body force
(a.k.a. right hand side)

Natural boundary
condition

Discrete matrix formulation

- Expressing variable (=pressure) inside element as the sum of the nodal values multiplied by weighting functions (= *standard Galerkin method*)



$$p(\mathbf{x}) = \sum_{i=1}^{3} p_i \psi_i$$

Discrete matrix formulation

- Taking weighting and test-functions to be the same:

$$p_i \int_\Omega (\mathbf{K}_{gw} \cdot \nabla \varphi_i) \cdot \nabla \varphi_j \, dV = \int_\Omega (\mathbf{K}_{gw} \cdot \mathbf{g} \rho_w) \cdot \nabla \varphi_j \, dV + \int_\Omega S_{gw} \, \varphi_j \, dV - \oint_{\partial\Omega} \mathbf{J}_{gw} \cdot \mathbf{n} \, \varphi_j \, dV$$

$$p_i \, M_{ij} = F_j - \oint_{\partial\Omega} \mathbf{J}_{gw} \cdot \mathbf{n} \, \varphi_j \, dV$$

Solution vector (p_i) | System matrix (M_{ij}) | Body force (F_j) | Natural boundary condition

Some simplifications

- Ignoring tensor-valued hydrological conductivity tensor (scalar diffusivity)

$$\mathbf{K}_{gw} = \mathbf{1}\,(k_{gw}/\mu_{\mathrm{H_2O}}) = \mathbf{1}\,K_{gw}$$

  - Where k_{gw} is the hydraulic conductivity

$$p_i \int_\Omega K_{gw}\,\nabla\varphi_i\cdot\nabla\varphi_j\,dV = \int_\Omega K_{gw}\rho_w\,\mathbf{g}\cdot\nabla\varphi_j\,dV + \int_\Omega S_{gw}\,\varphi_j\,dV - \oint_{\partial\Omega} \mathbf{J}_{gw}\cdot\mathbf{n}\,\varphi_j\,dV$$

```
Weight * K * MATMUL( dBasisdx,TRANSPOSE(dBasisdx))
```

```
Weight * K * rho * SUM( Gravity(1:DIM),dBasisdx))
```

Output of Variable

- We want to simply have the identity as variable (= solution):

$$\mathbf{J}_{gw} = \mathbf{K}_{gw} \cdot (\rho_w \mathbf{g} - \nabla p)$$

- We do the identiy component-wise:

$$J_i = K_{gw} \, (\rho_w \, g_i - \nabla_i p)$$

- Or in weak formulation:

$$\int_\Omega J_i \, dV = \int_\Omega K_{gw} \, (\rho_w g_i - \nabla_i p)$$

Discrete matrix formulation

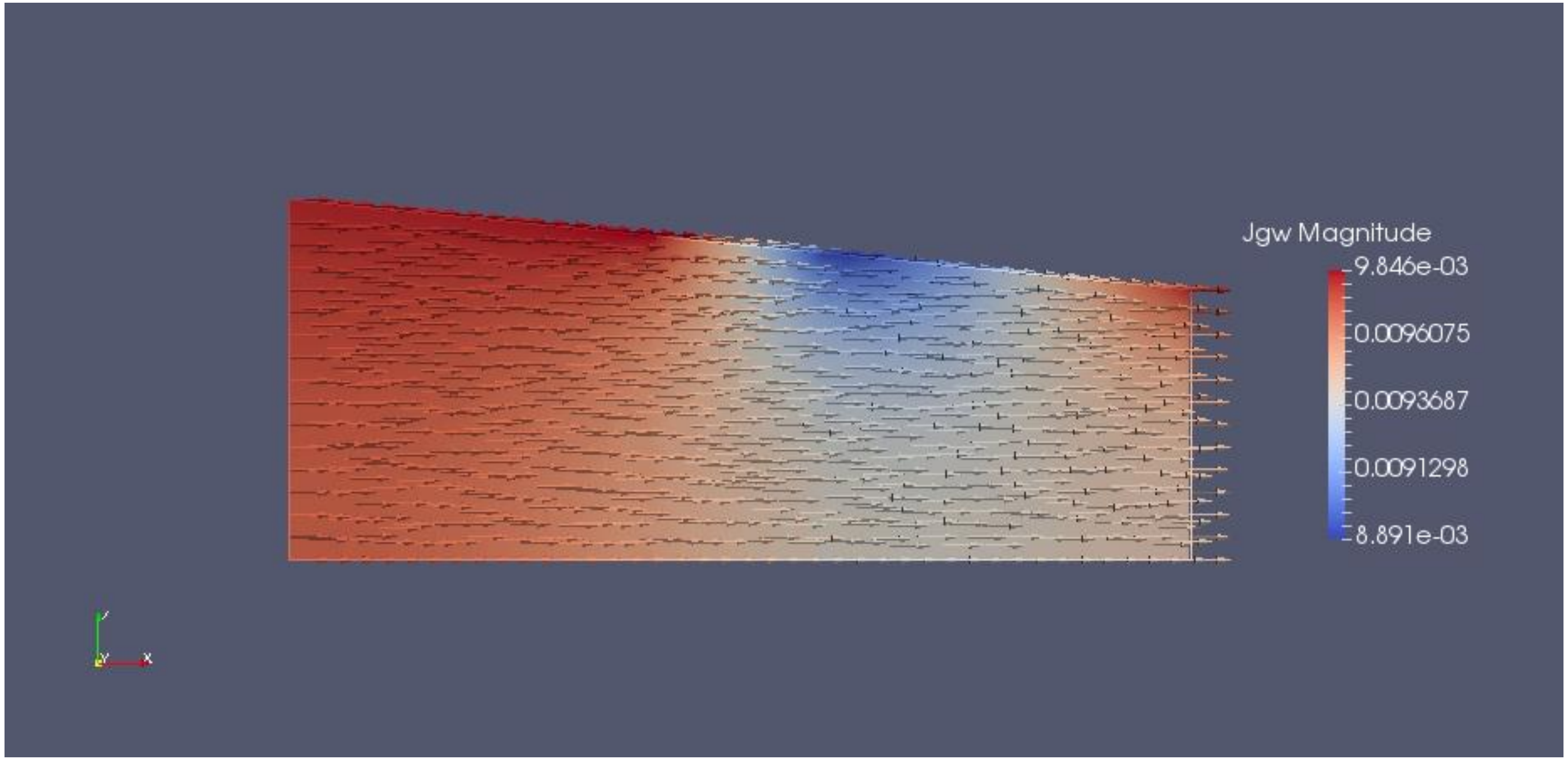
- Taking weighting and test-functions to be the same:

$$J_{\alpha,i} \int_{\Omega} \varphi_i \varphi_j \, dV = \int_{\Omega} K_{gw} \left(g_{\alpha} - \nabla_{\alpha} p \right) \varphi_j \, dV$$

$$J_i \, M_{ij} \qquad = \qquad F_j$$

Solution vector System matrix Body force

Darcy flux


Jgw Magnitude
9.846e-03
0.0096075
0.0093687
0.0091298
8.891e-03

Heat transfer

- With the computed flux, we want to advect/diffuse a temperature field

$$\bar{c\rho}\frac{\partial T}{\partial t} + \rho_w\, c_w \mathbf{J}_{gw} \cdot \nabla T = \nabla \cdot (\bar{\kappa} \nabla T)$$

Time derivative coefficient | convection coefficient | convection velocity | diffusion coefficient

```
Material 1
  Convection Velocity 1 = Equals Flux1
  Convection Velocity 2 = Equals Flux2
  Convection Velocity 3 = Equals Flux3
  time derivative coefficient = Real $porosity * waterheatcap * waterdens + (1.0 - porosity)*soilheatcap*soildens

  diffusion coefficient = Real $porosity * waterheatcon + (1.0 - porosity)*soilheatcon
  convection coefficient = Real $waterheatcap * waterdens
  reaction coefficient = Real 0.0
```

Heat transfer