Exercise Sheet No.8 — Deadline: 7. January 2014

EXERCISE 8 ADVECTION DISPERSION EQUATION

The instationary parabolic problem

$$\begin{aligned} \partial_t c + \nabla \cdot \big(-\tilde{D}\, \nabla c + c\, \vec{v} \big) &= 0 & \vec{x} \in \Omega \\ c &= f & \vec{x} \in \partial\Omega_D \\ \vec{n} \cdot \big(-\tilde{D}\, \nabla c + c\, \vec{v} \big) &= J_N & \vec{x} \in \partial\Omega_N \end{aligned}$$

is known as the Advection Dispersion equation with Dirichlet and Neumann boundary conditions. It describes coupled advective and dispersive transport of e.g. a solute in a porous medium. The velocity field $\vec{v}$ is given by *Darcy's Law*

$$\vec{v} = \frac{1}{\theta}\, \vec{j} = -\frac{1}{\theta}\, K\big(\nabla p - \rho g \vec{e}_z\big)$$

with the hydrostatic pressure p, the conductivity K and the porosity θ. Neglecting the hydromechanic dispersion and employing one of the *Millington-Quirk* models (see Soil Physics - Lecture Notes by Kurt Roth †), the effective dispersion coefficient $\tilde{D}$ may be expressed by the molecular diffusion coefficient D_m:

$$\tilde{D} = \theta^{4/3} D_m .$$

With c we denote the solute concentration in the carrier fluid with dimension $[c] = \frac{kg}{m^3}$.

In this exercise you will implement a discretization of the advection dispersion equation and apply it to a test problem. Following a common approach we discretize time and space separately. We therefore consider the equation to be an ordinary differential equation in time and employ a time stepping scheme. In this case we will restrict ourselves to the implicit Euler method:

For a given $c^0 \in C^2(\Omega)$ find $c^k \in C^2(\Omega)$:

$$\frac{c^{k+1} - c^k}{\tau} = \nabla \cdot \left(\tilde{D}\, \nabla c^{k+1} \right) - \nabla \cdot \left(c^{k+1}\, \vec{v} \right) \qquad k = 0 \ldots N-1$$

The discretization in space is given by the cell centered finite volume scheme. Hence, in time step k we require

$$\int_E c^{k+1} dV - \tau \int_{\partial E \setminus \partial\Omega_N} \tilde{D}\, \nabla c^{k+1}\, \vec{n}_E\, dA + \tau \int_{\partial E \setminus \partial\Omega_N} \vec{v} \left(c^{k+1}\Big|_* \right) \vec{n}_E\, dA = \int_E c^k dV - \tau \int_{\partial E \cap \partial\Omega_N} J_N\, dA$$

to hold for each cell E of the grid resolving the domain. $\vec{n}_E$ is the unit outer normal on $\partial\Omega_N$. Furthermore we require c^k to be piecewise constant on each cell and discretize the differential operators accordingly.

The evaluation of c^{k+1} within the advection term on a face e adjacent to the elements E and F may be achieved by choosing the upwind side for evaluation

$$c^{k+1}\Big|_* = \begin{cases} c^{k+1}\Big|_E & \text{if} \quad \vec{v} \cdot \vec{n}_E >= 0 \\ c^{k+1}\Big|_F & \text{otherwise} \end{cases} .$$

Implement a class `AdvectionDispersionAssembler` which assembles the system matrix of a single time step as given above. Its public interface should contain at least the following functions:

† v1.2, Spring 2007, on page 178, Equation (6.39). In the saturated zone, the porosity is the same as the volumetric water content.

- The Constructor:

```
AdvectionDispersionAssembler(
                       const Grid& grid,
                       const DispersionField& dispersion,
                       const AdvectionField& advection,
                       const BoundaryConditions& boundary_conditions
                       )
```

  The constructor requires references to the grid and boundary conditions object. The objects of type `DispersionField` and `AdvectionField` refer to parameter classes providing information about the effective dispersion and advection fields (see below).

- A function assembling the system matrix:

```
void assemble(
  Matrix& A,
  Vector& b,
  const Vector& x,
  const double tau,
  const bool upwinding = true
  )
```

  This function should assemble the system matrix `A` and right hand side `b` from the old solution `x` and the time step size τ. The last flag should switch whether or not upwinding is used for the advective term.

For the test problem, we refer to the two dimensional well setup as given in exercise no.6 (Model 3). For the total extraction rate of the well choose $q_w = 6 \cdot 10^{-4} \frac{m^2}{s}$. On the lower left boundary, we assume a contamination of the groundwater by a solute with $D_m = 2 \cdot 10^{-9} \frac{m^2}{s}$. Assuming $\theta = 0.3$ we find $\tilde{D} = 4 \cdot 10^{-10} \frac{m^2}{s}$. The contaminating reservoir maintains a constant concentration of $c_r = 1 \cdot 10^{-3} \frac{kg}{m^3}$ on the left boundary from $3\ m$ to $6\ m$ above the lower end of the confined aquifer. Neumann zero boundary conditions on all boundaries away from the contamination reservoir are applied.

Perform a simulation for 0.1 year following the beginning of the contamination (a day will be a good time step size).

Hint: If the color scaling in paraview is not set properly you might not be able to see the contamination plume. Before playing the movie it might be a good idea to scale the color using the output of the first time step. *5 Points*