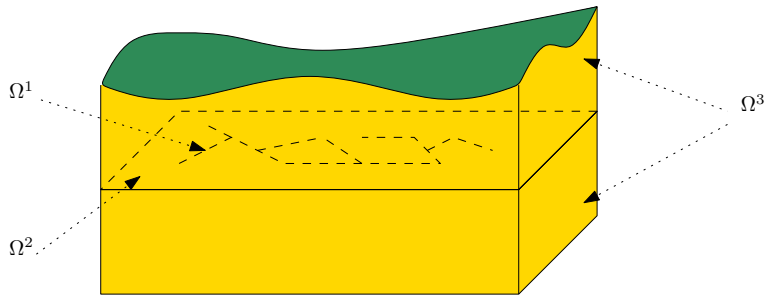
1 Model for transport of substances

Flow123d can simulate transport of substances dissolved in water. The transport mechanism is governed by the *advection*, and the *hydrodynamic dispersion*. Moreover the substances can move between ground and fractures.



1.1 Physical model

On the domain Ω^d of dimension $d \in \{1, 2, 3\}$, we consider a system of mass balance equations in the following form:

$$\partial_t(\vartheta c^i) + \operatorname{div}(\boldsymbol{q} c^i) - \operatorname{div}(\vartheta \mathbb{D}^i \nabla c^i) = F(c^1, \dots, c^s) \quad \text{on } \Omega^d. \tag{1}$$

The principal unknown is the concentration c^i $[kg\, m^{-3}]$ of a substance $i \in \{1, \dots, s\}$, which means weight of the substance in unit volume of the water. Other quantities are:

- ϑ $[-]$ is the porosity, i.e. fraction of space occupied by water and the total volume.
- $\boldsymbol{q}$ $[m\, s^{-1}]$ is the Darcy flux or the *macroscopic* water velocity. It is related to the *microscopic* water velocity $\boldsymbol{v}$ by the relation $\boldsymbol{q} = \vartheta \boldsymbol{v}$.
- The hydrodynamic dispersivity tensor $\mathbb{D}^i$ $[m^2 s^{-1}]$ has the form

  $$\mathbb{D}^i = D^i_m \tau \mathbb{I} + |\boldsymbol{v}|\big(\alpha^i_T \mathbb{I} + (\alpha^i_L - \alpha^i_T)\big)\frac{\boldsymbol{v} \times \boldsymbol{v}}{|\boldsymbol{v}|^2},$$

  which models (isotropic) molecular diffusion, and dispersion in longitudal and transversal direction to the flow. Here D^i_m $[m^2\, s^{-1}]$ is the molecular diffusion coefficient of the i-th substance (usual magnitude in clear water is 10^{-9}), $\tau = \vartheta^{1/3}$ is the tortuosity (by Millington and Quirk [1961]), α^i_L and α^i_T is the longitudal and the transversal dispersivity $[m]$, respectively.
- The reaction term $F(\dots)$ is currently neglected.

In lower dimensions $d = 1, 2$, equation (1) represents transport processes in planar or channel fractures whose cross-cut δ^d ($[m]$ for 2D and $[m^2]$ for 1D) is negligible with respect to the dimensions of the physical domain. For $d = 3$ we set $\delta^3 = 1$ $[-]$.

Boundary conditions. The physical boundary $\partial\Omega^d$ is decomposed into two parts:

$$\Gamma_D(t) = \{\boldsymbol{x} \in \partial\Omega^d \,|\, \boldsymbol{q}(t,\boldsymbol{x}) \cdot \boldsymbol{n}(\boldsymbol{x}) < 0\},$$
$$\Gamma_N(t) = \{\boldsymbol{x} \in \partial\Omega^d \,|\, \boldsymbol{q}(t,\boldsymbol{x}) \cdot \boldsymbol{n}(\boldsymbol{x}) \geq 0\},$$

where $\boldsymbol{n}$ stands for the unit outward normal vector to $\partial\Omega^d$. On the inflow part Γ_D, concentrations have to be prescribed (Dirichlet boundary condition):

$$c^i(t,\boldsymbol{x}) = c^i_D(t,\boldsymbol{x}) \text{ on } \Gamma_D(t),$$

while on Γ_N we impose homogeneous Neumann boundary condition:

$$-\mathbb{D}^i(t,\boldsymbol{x})\nabla c^i(t,\boldsymbol{x}) \cdot \boldsymbol{n}(\boldsymbol{x}) = 0 \text{ on } \Gamma_N(t).$$

Communication between dimensions. Transport of substances is considered also on interfaces of physical domains with adjacent dimensions (i.e. 3D-2D and 2D-1D, but not 3D-1D). Denoting c_{d+1}, c_d the concentration of a given substance in Ω^{d+1} and Ω^d, respectively, the comunication on the interface between Ω^{d+1} and Ω^d is described by:

$$q^c = \sigma^c(c_{d+1} - c_d) + \begin{cases} q^w c_{d+1} & \text{if } q^w \geq 0, \\ q^w c_d & \text{if } q^w < 0, \end{cases} \tag{2}$$

where

- q^c $[kg\, m^{-2}\, s^{-1}]$ is the concentration flux from Ω^{d+1} to Ω^d,
- σ^c $[m\, s^{-1}]$ is a transition parameter,
- q^w $[m\, s^{-1}]$ is the water flux from Ω^{d+1} to Ω^d.

Equation (2) is incorporated as a boundary condition for the problem on Ω^{d+1}:

$$-\mathbb{D}\nabla c_{d+1} \cdot \boldsymbol{n} + q^w c_{d+1} = q^c$$

and a source term in Ω^d:

$$F^c_d = \frac{\delta_{d+1}}{\delta_d}(\sigma^c + |q^w|)(c_{d+1} - c_d).$$

2 Numerical solution

For the numerical approximation of the advection-diffusion equation (1) we distinguish whether diffusion is present or not. Since the true solution has qualitatively different properties, we also choose different numerical methods for each case.

2.1 Pure advection

2.2 Advection with diffusion

For the general case we use the discontinuous Galerkin space approximation and implicit Euler time discretization. Let τ, h be the time step and the space discretization parameter, respectively. We assume that $\mathcal{T}_h^d$ is a regular partition of the domain Ω^d into simplices, $d = 1, 2, 3$. We define the set $\mathcal{E}_h^d$ of all edges of elements in $\mathcal{T}_h$ (triangles for $d = 3$, line segments for $d = 2$ and points for $d = 1$). Further, $\mathcal{E}_{h,I}^d$ will denote interior edges, $\mathcal{E}_{h,D}^d$ edges that coincide with Γ_D^d and $\mathcal{E}_{h,C}^d$ stands for edges on interface with Ω^{d-1}.

Let us fix one substance and the space dimension d. At each time instant we search for the concentration field $c_d^h \in V_d^h$, where

$$V_d^h = \{v : \overline{\Omega^d} \to \mathbb{R} \,|\, v_{|T} \in P_1(T)\ \forall T \in \mathcal{T}_h^d\}$$

is the space of functions piecewise affine on the elements of $\mathcal{T}_h^d$, possibly discontinuous across the element interfaces. The discrete problem reads:

$$\left(\vartheta \frac{c_d^h - c_{d,old}^h}{\tau}, v\right)_{\Omega^d} + a_d^h(c_d^h, v) = b_d^h(v) \quad \forall v \in V_d^h.$$

Here $c_{d,old}^h$ is the solution from the previous time step and the forms a_d^h, b_d^h are defined as follows:

$$\begin{aligned} a_d^h(u,v) = {} & (\vartheta \mathbb{D}\nabla u, \nabla v)_{\Omega^d} + ((\operatorname{div} \boldsymbol{q})u, v)_{\Omega^d} + (\boldsymbol{q}\cdot\nabla u, v)_{\Omega^d} \\ & - \vartheta \sum_{E\in\mathcal{E}_{h,I}^d} \left((\{\mathbb{D}\nabla u\}_\omega \cdot \boldsymbol{n}, [v])_E + (\{\mathbb{D}\nabla v\}_\omega \cdot \boldsymbol{n}, [u])_E \right) \\ & - \sum_{E\in\mathcal{E}_{h,I}^d} (\boldsymbol{q}\cdot\boldsymbol{n}\{v\}_\omega, [u])_E + \sum_{E\in\mathcal{E}_{h,I}^d} \gamma_E ([u],[v])_E + \sum_{E\in\mathcal{E}_{h,D}^d} \gamma_E (u,v)_E, \end{aligned}$$

$$b_d^h(v) = \sum_{E\in\mathcal{E}_{h,D}^d} \gamma_E (c_D, v)_E.$$

For an interior edge E we denote by $T^-(E)$ and $T^+(E)$ the elements sharing E. By $\boldsymbol{n}$ we mean the unit normal vector to E pointing from $T^-(E)$ towards $T^+(E)$, the inter-element jump is defined as $[f] = f_{|T^-(E)} - f_{|T^+(E)}$, and $\{f\}_\omega = \omega f_{|T^-(E)} + (1-\omega) f_{|T^+(E)}$ denotes a weighted average of the quantity f. The weight ω is chosen in a specific way (see Ern et al. [2009] for details) taking into account possible inhomogeneity of $\mathbb{D}$. The stabilization parameter $\gamma_E > 0$ is user dependent; its value affects the inter-element jumps of the solution.

If there are interfaces between adjacent dimensions, then the following terms are added to the left and right hand side, respectively:

$$a_{d,com}^h(u,v) = \sum_{E\in\mathcal{E}_{h,C}^d} (\sigma^c + (q^w)^-)(u,v)_E - \sum_{T\in\mathcal{T}_h^d\cap\mathcal{E}_{h,C}^{d+1}} (\sigma^c + |q^w|)(u,v)_T,$$

$$b_{d,com}^h(v) = \sum_{E\in\mathcal{E}_{h,C}^d} (\sigma^c + (q^w)^-)(c_{d-1}^h, v)_E - \sum_{T\in\mathcal{T}_h^d\cap\mathcal{E}_{h,C}^{d+1}} (\sigma^c + |q^w|)(c_{d+1}^h, v)_T.$$

Here we obviously set $\mathcal{E}_{h,C}^4 = \mathcal{E}_{h,C}^1 = \emptyset$.

References

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