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FLOW123D - draft, scheme of new inputs

version 1.7.0

**Documentation of file formats
and brief user manual.**

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Chapter 1

Quick start

Flow123D is a software for simulation of water flow and reactionary solute transport in a heterogeneous porous and fractured medium. In particular it is suited for simulation of underground processes in a granite rock massive. The program is able to describe explicitly processes in 3D medium, 2D fractures, and 1D chanels and exchange between domains of different dimension. The computational mesh is therefore collection of 3D tetrahedrons, 2D triangles and 1D line segments.

The water flow model assumes a saturated medium described by Darcy law. For discretization, we use lumped mixed-hybrid finite element method. We support both steady and unsteady water flow.

The solute transport model can deal with several dissolved substances. It contains non-equilibrium dual porosity model, i.e. exchange between mobile and immobile pores. There is also model for several types of adsorption in both the mobile and immobile zone. The implemented adsorption models are linear adsorption, Freundlich isotherm and Langmuir isotherm. The solute transport model uses finite volume discretization with up-winding in space and explicit Euler discretization in time. The dual porosity and the adsorption are introduced into transport by operator splitting. The dual porosity model use analytic solution and the non-linear adsorption is solved numerically by the Newton method.

Reaction between transported substances can be modeled either by a SEMCHEM module, which is slow, but can describe all sorts of reactions. On the other hand, for reactions of the first order, i.e. linear reactions or decays, we provide our own solver which is much faster. Reactions are coupled with transport by the operator splitting method,

The program provides output of the pressure, the velocity and the concentration fields in two file formats. You can use file format of GMSH mesh generator and post-processor or you can use output into widely supported VTK format. In particular we recommend Paraview software for visualization and post-processing of VTK data.

The program is implemented in C/C++ using essentially PETSC library for linear algebra. The water flow as well as the transport simulation and reactions can be computed in parallel using MPI environment.

The program is distributed under GNU GPL v. 3 license and is available on the project web page: http://dev.nti.tul.cz/trac/flow123d

1.1 Basic usage

1.1.1 How to run the simulation.

On the Linux system the program can be started either directly or through a script `flow123d.sh`. When started directly, e.g. by the command

```
> flow123d -s example.ini
```

the program requires one argument after switch `-s` which is the name of the principal input file. Full list of possible command line arguments is as follows.

format using particular macros.

`--help`
: Parameters interpreted by Flow123d.Remaining parameters are passed to PETSC.

`-s, --solve` *file*
: Set principal CON input file. All relative paths in the CON file are relative against current directory.

`-i, --input_dir` *directory*
: The place holder `${INPUT}` used in the path of an input file will be replaced by given *directory*.

`-o, --output_dir` *directory*
: All paths for output files will be relative to this *directory*.

`-l, --log` *file_name*
: Set base name of log files.

`--no_log`
: Turn off logging.

`--no_profiler`
: Turn off profiler output.

`--full_doc`
: Prints full structure of the main input file.

`--JSON_template`
: Prints description of the main input file as a valid CON file template.

All other parameters will be passed to the PETSC library. An advanced user can influence lot of parameters of linear solver. In order to get list of supported options use parameter `-help` together with some valid input. Options for various PETSC modules are displayed when the module is used for the first time.

Alternatively, you can use script `flow123d.sh` to start parallel jobs or limit resources used by the program. This script accepts the same parameters as the program itself and further following additional parameters:

-h
Usage overview.

-t *timeout*
Upper estimate for real running time of the calculation. Kill calculation after *timeout* seconds. Can also be used by PBS to choose appropriate job queue.

-np *number of processes*
Specify number of parallel processes for calculation.

-m *memory limit*
Limits total available memory to *memory limit* bytes.

-n *priority*
Change (lower) priority for the calculation. See `nice` command.

-r *out file*
Stdout and stderr will be redirected to *out file*.

On the Windows system we use Cygwin libraries in other to emulate Linux API. Therefore you have to keep the Cygwin libraries within the same direcotry as the program executable. The Windows package that can be downloaded from project web page contains both the Cygwin libraries and the mpiexec command for starting parallel jobs on the Windows workstations.

Then you can start the sequential run by the command:

```
> flow123d.exe -s example.ini
```

or the parallel run by the command:

```
> mpiexec.exe -np 2 flow123d.exe -s example.ini
```

The program accepts the same parameters as the Linux version, but there is no script similar to `flow123d.sh` for the Windows system.

1.1.2 Tutorial problem

CON file format

The main input file use slightly extended JSON file format which together with some particular constructs forms a CON (C++ object notation) file format. Main extensions of the JSON are unquoted key names (as long as they do not contain whitespaces), possibility to use `=` instead of `:` and C++ comments, i.e. `//` for the one line and `/* */` for the multi-line comment. In CON file format, we prefere to call JSON objects as "records" and we introduce also "abstract records" that mimics C++ abstract classes, the arrays of an CON file have only alements of the same type (possibly using abstract record types for polymorphism). The usual keys are in lower case and without spaces (using underscores instead), there are few special upper case keys that are interpreted by the reader: `REF` key for references, `TYPE` key for specifing actual type of an abstract record. For detailed description see Section 3.1.2.

Geometry

In the following, we shall provide commented input for the tutorial problem (`tests/03_transport_small_`
We consider simple 2D problem with a branching 1D fracture (see Figure 1.1 for the geometry). To prepare the mesh file we use the GMSH software. First, we construct the geometry file. In our case the geometry consists of:

- one physical 2D domain corresponding to the whole square
- three 1D physical domains of the fracture
- four 1D boundary physical domains of the 2d domain
- three 0D boundary physical domains of the 1d domain

In this simple example, we can in fact combine physical domains in every group, however we use this more complex setting for demonstration purposes. Using GMSH graphical interface we can prepare the GEO file where physical domains are referenced by numbers, then we use any text editor and replace numbers with string labels in such a way that the labels of boundary physical domains start with the dot character. These are the domains where we would not do any calculations but use them for setting boundary conditions. Finally, we get the GEO file like this:

```
1  cl1 = 0.16;
2  Point(1) = {0, 1, 0, cl1};
3  Point(2) = {1, 1, 0, cl1};
4  Point(3) = {1, 0, 0, cl1};
5  Point(4) = {0, 0, 0, cl1};
6  Point(6) = {0.25, -0, 0, cl1};
7  Point(7) = {0, 0.25, 0, cl1};
8  Point(8) = {0.5, 0.5, -0, cl1};
9  Point(9) = {0.75, 1, 0, cl1};
10 Line(19) = {9, 8};
11 Line(20) = {7, 8};
12 Line(21) = {8, 6};
13 Line(22) = {2, 3};
14 Line(23) = {2, 9};
15 Line(24) = {9, 1};
16 Line(25) = {1, 7};
17 Line(26) = {7, 4};
18 Line(27) = {4, 6};
19 Line(28) = {6, 3};
20 Line Loop(30) = {20, -19, 24, 25};
21 Plane Surface(30) = {30};
22 Line Loop(32) = {23, 19, 21, 28, -22};
23 Plane Surface(32) = {32};
24 Line Loop(34) = {26, 27, -21, -20};
25 Plane Surface(34) = {34};
26 Physical Point(".1d_top") = {9};
27 Physical Point(".1d_left") = {7};
28 Physical Point(".1d_bottom") = {6};
29 Physical Line("1d_upper") = {19};
30 Physical Line("1d_lower") = {21};
31 Physical Line("1d_left_branch") = {20};
32 Physical Line(".2d_top") = {23, 24};
33 Physical Line(".2d_right") = {22};
34 Physical Line(".2d_bottom") = {27, 28};
35 Physical Line(".2d_left") = {25, 26};
36 Physical Surface("2d") = {30, 32, 34};
```

Notice the labeled physical domains on lines 26 – 36. Then we just set the discretization step `cl1` and use GMSH to create the mesh file. The mesh file contains as the 'bulk' elements where we perform calculations as the 'boundary' elements (on boundary physical domains) where we only set boundary conditions.

Having the computational mesh, we can create the main input file with description of our problem.

```
{
  problem = {
    TYPE = "SequentialCoupling",
    description = "Transport 1D-2D, (convection, dual porosity, sorption)",
    mesh = {
      mesh_file = "./input/mesh_with_boundary.msh",
      sets = [
          { name="1d_domain",
            region_labels = [ "1d_upper", "1d_lower", "1d_left_branch" ]
          }
        ]
    },
```

The file starts with particular problem type, currently the type "SequantialCoupling" is suported, and textual problem description. Next, we specify the computational mesh, here it consists of the name of the mesh file and declaration of one *region set* composed of all 1D regions i.e. representing the whole fracture. Other keys of the mesh record allows lebeling regions given only by numbers, defining new regions in terms of element numbers (e.g to have leakage on single element), defining boundary regions, and set operations with region sets, see Section **??** for details.

Flow setting

Next, we setup the flow problem. We shall consider a flow driven only by the pressure gradient (no gravity), setting the Dirichlet boundary condition on the whole boundary with the pressure head equal to $x+y$. The conductivity will be 1 on the 2D domain and 10 on the 1D domain. The fracture width will be $\delta_1 = 1$ (quite unnatural) as well as the transition parameter $\sigma_2 = 1$ which describes a "conductivity" between dimensions. These are currently the default values.

```
    primary_equation = {
      TYPE = "Steady_MH",

      bulk_data = [
        { r_set = "1d_domain", conductivity = 10 },
        { region = "2d",       conductivity = 1  }
      ],

      bc_data = [
        { r_set = "BOUNDARY",
          bc_type = "dirichlet",
          bc_pressure = { TYPE="FieldFormula", value = "x+y" }
        }
      ],

```

```
28        output = {
29          output_stream = { REF = "/system/output_streams/0" },
30          pressure_p0 = "flow_output_stream",
31          pressure_p1 = "flow_output_stream",
32          velocity_p0 = "flow_output_stream"
33        },
34
35        solver = { TYPE = "Petsc", accuracy = 1e-07 }
36      }, // primary equation
```

On line 11, we specify particular implementation (numerical method) of the flow solver, in this case the Mixed-Hybird solver for unsteady probelems. On lines 16 – 19, we set mathematical fields that lives on the computational domain (i.e. the bulk domain), we set only the conductivity field since other bulk fields has appropriate default values. On lines 21 – 26, we set fields for boundary conditions. We use implicitely defined set "BOUNDARY" that contains all boundary regions and set there dirichlet boundary condition in terms of the pressure head. In this case, the field is not of the implicit type "FieldConstant", so we must specify the type of the field "FieldFormula". Se Section **??** for other boundary fields. On lines 28 – 33, we specify which output fields should be written into which output stream (that means particular output file, with given format). Currently, we support only one output stream per equation, so this allows at least switching individual output fields on or off. Notice the reference used on line 29 pointing to the definition of the output streams at the end of the file. Finally, we specify type of the linear solver and its tolerance.

Transport setting

We also consider subsequent transport problem with the porosity $\theta = 0.25$ and zero initial concentration. The boundary condition is equal to 1 and is automatically applied only on the inflow part of the boundary. There is also some adsorption and dual porosity model in this particular test case, but we do not discuss this topic here for the sake of simplicity, see Section **??** for the description.

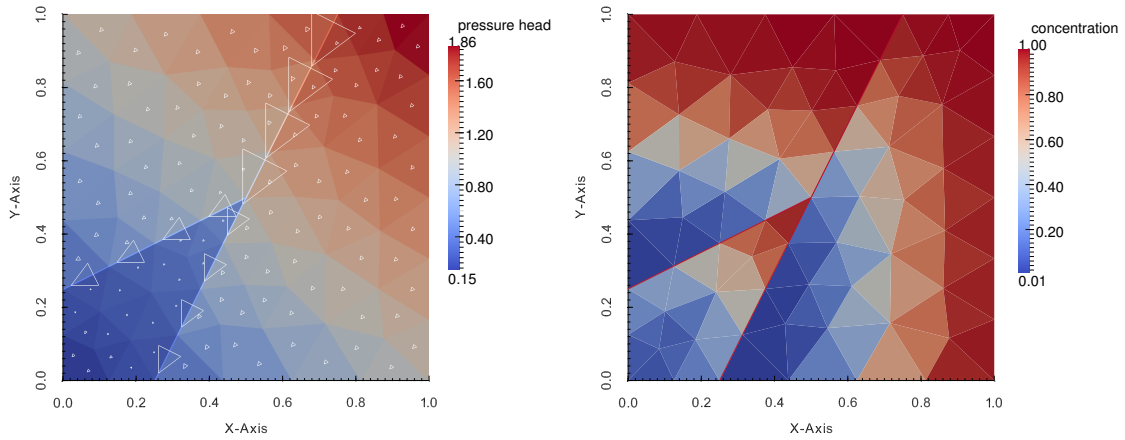
```
37      secondary_equation = {
38       TYPE = "TransportOperatorSplitting",
39
40       dual_porosity = true,
41       sorption_enable = true,
42       substances = [ "age", "U235" ],
43
44       bulk_data = [
45         { r_set = "ALL",
46           init_conc = 0,
47           por_m = 0.25,
48           por_imm = 0.25,
49           alpha = [0.01, 0.01],
50           phi = 0.5,
51           sorp_type = [1, 2],
```

```
52            sorp_coef0 = [0.02, 0.02],
53            sorp_coef1 = [0, 0.5]
54          }
55        ],
56
57        bc_data = [
58          { r_set = "BOUNDARY",
59            bc_conc = 1.0
60          }
61        ],
62
63        output = {
64          output_stream = { REF = "/system/output_streams/1" },
65          save_step = 0.01,
66          mobile_p0 = "transport_output_stream"
67        },
68
69        time = { end_time = 1.0 }
70      } // secondary_equation
71    }, // problem
```

For the transport problem we use implementation called "TransportOperatorSplitting" which is explicit finite volume solver of the convection equation (without diffusion), the operator splitting is used for the equilibrium adsorption as well as for the dual porosity model. Both these are switched on as we can see on lines 40, 41. On the next line, we set names of transported substances, here it is the age of the water and the uranium 235. On lines 44 – 55, we set the bulk fields in particular the porosity 'por_m' and the initial concentrations (one for every substance). However, on line 46, we see only single value since an automatic conversion is applied to turn the scalar zero into the zero vector (of size 2). On line 53, we can see vector that set different adsorption coefficients for the two substances. Then, on lines 57 – 61, we set the boundary fields namely the concentration on the inflow part of the boundary. We need not to specify type of the condition since currently this is the only one available. In the output record we have to specify the save step (line 65) for the output fields. And finally, we have to set the time setting, here only the end time of the simulation since the step size is determined from the CFL condition, however you can set smaller time step if you want.

Output streams and results

```
72    system = {
73      output_streams = [
74        {
75          file = "test3.pvd",
76          format = { TYPE = "vtk", variant = "ascii" },
77          name = "flow_output_stream"
78        },
79        {
80          file = "test3-transport.pvd",
```



(a) Elementwise pressure head and velocity field (triangles).

(b) Propagation of U235 from the inflow part of the boundary.

Figure 1.1: Results of the tutorial problem.

```
81          format = { TYPE = "vtk", variant = "ascii" },
82          name = "transport_output_stream"
83        }
84      ]
85    }
86  }
```

The end of the input file contains declaration of two output streams, on for the flow problem and one for the transport problem. Currently, we support output into VTK format and GMSH data format. On Figure 1.1 you can see the results, the pressure and the velocity field on the left and the concentration of U235 at time $t = 0.9$ on the right. Even if the pressure gradient is the same on the 2D domain as on the fracture, the velocity field is ten times faster on the fracture. Since porosity is same, the substance is transported faster by the fracture and then appears in the bottom left 2D domain before the main wave propagating solely through the 2D domain.

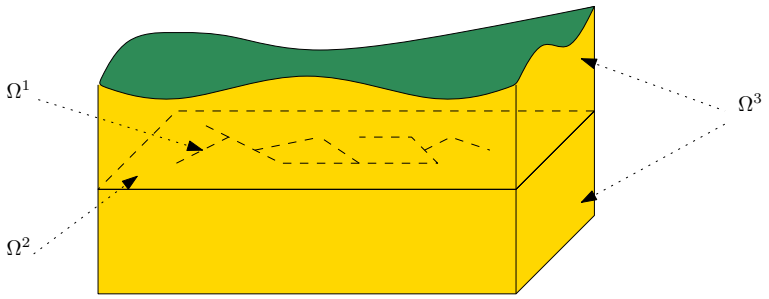
The output files can be either `*.msh` files accepted by the GMSH or one can use VTK format that can be post-processed by Paraview.

In the following chapter, we briefly describe structure of individual input files in particular the main INI file. In the last chapter, we describe mathematical models and numerical methods used in the Flow123d.

Chapter 2

Mathematical models of physical reality

Flow123d provides models for Dary flow in porous media as well as for the transport and reactions of soluted substances. In this section, we describe mathematical formulations of these models together with physical meaning and units of all involved quantities. Common and unique feature of all models is support of domains with mixed dimension. Let $\Omega_3 \subset \mathbf{R}^3$ be an open set representing continuum approximation of porous and fractured medium. Similarly, we consider open set $\Omega_2 \subset \mathbf{R}^2$ representing 2D fractures and open set $\Omega_1 \subset \mathbf{R}^3$ of 1D channels or preferential paths (see Fig ??). We assume that Ω_2 and Ω_1 are polygonal. For every dimension $d = 1, 2, 3$, we introduce a triangulation $\mathcal{T}_d$ of the open set Ω_d that consists of finite elements T_d^i, $i = 1, \ldots, N_E^d$. The elements are simplexes that is tetrahedrons, triangles and lines.



Present numerical methods requires meshes satisfying the compatibility conditions

$$T_{d-1}^i \cap T_d \subset \mathcal{F}_d, \qquad \text{where } \mathcal{F}_d = \bigcup_k \partial T_d^k \tag{2.1}$$

and

$$T_{d-1}^i \cap \mathcal{F}_d \text{ is either } T_{d-1}^i \text{ or } \emptyset \tag{2.2}$$

for every $i \in \{1, \ldots, N_E^{d-1}\}$, $j \in \{1, \ldots, N_E^d\}$, and $d = 2, 3$. That is the $(d-1)$-dimensional elements are either between d-dimensional elements and match their sides or they poke out of Ω_d.

2.1 Darcy flow model

We consider simplest model for the velocity of the steady or unsteady flow in porous and fractured medium given by Darcy low:

$$\boldsymbol{w} = -\mathbb{K}\nabla H \quad \text{on } \Omega_d, \text{ for } d = 1, 2, 3. \tag{2.3}$$

We drop the dimension index of quantities in equations if it is same as the dimension of the set where the equation holds. In (2.3), $\boldsymbol{w}_d$ [ms^{-1}] is the superficial velocity, $\mathbb{K}_d$ is the conductivity tensor, and H_d [m] is the piezometric head. The velocity is related to the flux $\boldsymbol{q}_d$ with units [m^{4-d}s^{-1}] through

$$\boldsymbol{q}_d = \delta_d \boldsymbol{w}_d.$$

where δ_d [m^{3-d}] is a cross section coefficient, in particular $\delta_3 = 1$, δ_2 [m] is the thickness of a fracture, and δ_1 [m^2] is the cross-section of a channel. The flux q_d is the volume of the liquid (water) that pass through a unit square ($d = 3$), unit line ($d = 2$), or through a point ($d = 1$) per one second. The conductivity tensor is given by the product $\mathbb{K}_d = k_d \mathbb{A}_d$, where $k_d > 0$ is the hydraulic conductivity [ms^{-1}] and A_d is $3x3$ dimensionless anisotropy tensor which has to be symmetric and positive definite. The piezometric-head H_d has units [m] and is related to the pressure head h_d by $H_d = h_d + z$ assuming that the gravity force acts in negative direction of the z-axes. Combining these relations we get Darcy low in the form:

$$\boldsymbol{q} = -\delta k \mathbb{A} \nabla (h + z) \qquad \text{on } \Omega_d, \text{ for } d = 1, 2, 3. \tag{2.4}$$

Next, we employ continuity equation for saturated porous medium:

$$\partial_t (S\, h) + \operatorname{div} \boldsymbol{q} = F \qquad \text{on } \Omega_d, \text{ for } d = 1, 2, 3, \tag{2.5}$$

where S_d is the storativity and F_d is a source term. In our setting the principal unknowns of the system (2.4, 2.5) are the pressure head h_d and the flux $\boldsymbol{q}_d$.

The storativity $S_d > 0$ or the volumetric specific storage [m^{-1}] can be expressed as

$$S_d = \gamma_w (\beta_r + \nu \beta_w), \tag{2.6}$$

where γ_w [kgm^{-2}s^{-2}] is the specific weight of water, ν is the porosity [$-$], β_r is compressibility of the bulk material of the pores (rock) and β_w is compressibility of the water both with units [kg^{-1}ms^{-2}]. For steady problems we set $S_d = 0$ for all dimensions $d = 1, 2, 3$. The source term F_d [m^{3-d}s^{-1}] on the right hand side of (2.5) consists of the volume density of prescribed sources f_d [s^{-1}] and flux from higher dimension. Exact formula is slightly different for every dimension and will be discussed presently.

On Ω_3 we simply have $F_3 = f_3$ [s^{-1}].

On the set $\Omega_2 \cap \Omega_3$ the fracture is surrounded by one 3D surface from every side (or just one surface since we allow also 2D models on the boundary). On $\partial\Omega_3 \cap \Omega_2$ we prescribe boundary condition of Robin type

$$\begin{aligned} \boldsymbol{q}_3 \cdot \boldsymbol{n}^+ &= q_{32}^+ = \sigma_3^+ (h_3^+ - h_2), \\ \boldsymbol{q}_3 \cdot \boldsymbol{n}^- &= q_{32}^- = \sigma_3^- (h_3^- - h_2), \end{aligned}$$

where $\boldsymbol{q}_3 \cdot \boldsymbol{n}^{+/-}$ [ms^{-1}] is the outflow from Ω_3, $h_3^{+/-}$ is a trace of the pressure head on Ω_3, h_2 is the pressure head on Ω_2, and $\sigma_3^{+/-} = \sigma_{32}$ [s^{-1}] is the transition coefficient that will be discussed later. On the other hand, the sum of the interchange fluxes $\boldsymbol{q}_{32}^{+/-}$ forms a volume source on Ω_2. Therefore F_2 [ms^{-1}] on the right hand side of (2.5) is given by

$$F_2 = \delta_2 f_2 + (q_{32}^+ + q_{32}^-). \tag{2.7}$$

The communication between Ω_2 and Ω_1 is similar. However, in the 3D ambient space, an 1D channel can join multiple 2D fractures $1, \ldots, n$. Therefore, we have n independent outflows from Ω_2:

$$\boldsymbol{q}_2 \cdot \boldsymbol{n}^i = q_{21}^i = \sigma_2^i (h_2^i - h_1),$$

where $\sigma_2^i = \delta_2^i \sigma_{21}$ [ms^{-1}] is the transition coefficient integrated over the width of the fracture i. Sum of the fluxes forms part of F_1 [m^{2}s^{-1}]

$$F_1 = \delta_1 f_1 + \sum_i q_{21}^i. \tag{2.8}$$

The transition coefficients σ_d [m^{3-d}s^{-1}] are independent parameters in our setting however in practice they should be related to the conductivity in direction (or plane) perpendicular to the fracture (channel). According to [4] one can use

$$\sigma_3 = \frac{2\mathbb{K}_2 : \boldsymbol{n}_2 \otimes \boldsymbol{n}_2}{\delta_2}, \sigma_2^i = \frac{2\delta_2 \mathbb{K}_1 : \boldsymbol{n}_1^i \otimes \boldsymbol{n}_1^i}{\delta_1}$$

where $\boldsymbol{n}_2$ is normal to the fracture (sign doesn't matter) and $\boldsymbol{n}_1^i$ is normal to the channel that is tangential to the fracture i.

In order to obtain unique solution we have to prescribe boundary conditions. Currently we support three basic types of boundary condition. Consider disjoint decomposition of the boundary

$$\partial\Omega_d = \Gamma_d^D \cap \Gamma_d^N \cap \Gamma_d^R$$

into Dirichlet, Neumann, and Robin parts. We prescribe

$$h_d = h_d^D \qquad \text{on } \Gamma_d^D, \tag{2.9}$$

$$\boldsymbol{q}_d \cdot \boldsymbol{n} = q_d^N \qquad \text{on } \Gamma_d^N, \tag{2.10}$$

$$\boldsymbol{q}_d \cdot \boldsymbol{n} = \sigma_d^R (h_d - h_d^R) \qquad \text{on } \Gamma_d^R. \tag{2.11}$$

where h_d^D, h_d^R is the prescribed pressure head [m], which alternatively can be prescribed through the piezometric head H_d^D, H_d^R respectively. q_d^N is the prescribed surface density of the boundary outflow [m^{4-d}s^{-1}], and σ_d^R is the transition coefficient [m^{3-d}s^{-1}]. The problem is well posed only if there is Dirichlet or Robin boundary condition on every component of the set $\Omega_1 \cup \Omega_2 \cup \Omega_3$ and $\sigma_d > 0$ for $d = 2, 3$.

For unsteady problems one has to specify initial condition in terms of initial pressure head h_d^0 or initial piezometric head H_d^0.

2.2 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.

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

$$\delta_d \partial_t(\vartheta c^i) + \operatorname{div}(\boldsymbol{q}_d c^i) - \operatorname{div}(\vartheta \delta_d \mathbb{D}^i \nabla c^i) = F_S + F_C(c^i) + F_R(c^1, \dots, c^s). \tag{2.12}$$

The principal unknown is the concentration c^i [kgm^{-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.
- The hydrodynamic dispersivity tensor $\mathbb{D}^i$ [m^{2}s^{-1}] has the form

$$\mathbb{D}^i = D_m^i \tau \mathbb{I} + |\boldsymbol{v}| \left(\alpha_T^i \mathbb{I} + (\alpha_L^i - \alpha_T^i) \frac{\boldsymbol{v} \times \boldsymbol{v}}{|\boldsymbol{v}|^2} \right),$$

  which represents (isotropic) molecular diffusion, and mechanical dispersion in longitudal and transversal direction to the flow. Here D_m^i [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 [5]), α_L^i [m] and α_T^i [m] is the longitudal dispersivity and the transversal dispersivity, respectively. Finally, $\boldsymbol{v}$ [ms^{-1}] is the *microscopic* water velocity, related to the Darcy flux $\boldsymbol{q}_d$ by the relation $\boldsymbol{q}_d = \vartheta \delta_d \boldsymbol{v}$. The value of D_m^i for specific substances can be found in literature (see e.g. [1]). For instructions on how to determine α_L^i, α_T^i we refer to [2, 3].
- F_S [kgm^{-d}s^{-1}] is the density of concentration sources.
- $F_C(c^i)$ [kgm^{-d}s^{-1}] is the density of concentration sources due to exchange between regions with different dimensions, see (2.15) below.
- The reaction term $F_R(\dots)$ [kgm^{-d}s^{-1}] is currently neglected.

Initial and boundary conditions. At time $t = 0$ the concentration is determined by the initial condition

$$c^i(0, \boldsymbol{x}) = c_0^i(\boldsymbol{x}).$$

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, the user must provide Dirichlet boundary condition for concentrations:

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

while on Γ_N we impose homogeneous Neumann boundary condition:

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

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:

$$q^c = \delta_{d+1}\sigma^c(\vartheta_{d+1}c_{d+1} - \vartheta_d c_d) + \begin{cases} q^w c_{d+1} & \text{if } q^w \geq 0, \\ q^w c_d & \text{if } q^w < 0, \end{cases} \tag{2.13}$$

where

- q^c [kgm^{-d}s^{-1}] is the density of concentration flux from Ω_{d+1} to Ω_d,
- σ^c [ms^{-1}] is a transition parameter. Its nonzero value causes mass exchange between dimensions whenever the concentrations differ. It is recommended to set either $\sigma^c = 0$ (exchange due to water flux only) or, similarly as in (2.1),

$$\sigma^c \approx \frac{\delta_{d+1}}{\delta_d}\mathbb{D} : \boldsymbol{n} \otimes \boldsymbol{n}.$$

- q^w [m^{3-d}s^{-1}] is the water flux from Ω_{d+1} to Ω_d, i.e. $q^w = \boldsymbol{q}_{d+1} \cdot \boldsymbol{n}_{d+1}$.

Equation (2.13) is incorporated as the total flux boundary condition for the problem on Ω_{d+1} and a source term in Ω_d:

$$-\vartheta\delta_{d+1}\mathbb{D}\nabla c_{d+1} \cdot \boldsymbol{n} + q^w c_{d+1} = q^c, \tag{2.14}$$

$$F_C^d = q^c. \tag{2.15}$$

Chapter 3

File formats

3.1 Input files

In this section we shall describe whole structure of the program input, namely the structure of the root input file. File formats of other files used for input of the mesh or large field data (e.g. the GMSH file format) are described in separate sections. The program input consists of the root input file given as the parameter on the command line and possibly several other files with large input data. The root input file is in so called CON file format that is a slight extension of the JSON file format.

In this section we shall describe format of the input files. At first, we specify syntax of an extension to the JSON file format. Then we set rules for input of more specific data constructs. We continue by description of general scheme for input of boundary conditions and material time-space variable data. And finally, we describe setting of particular equations and their solvers.

The aim of this draft is twofold. First, we want to outline the way how to translate current input file format (in version 1.6.5) into the new one without extending the existing functionality. Second, we want to propose a new way how to input general boundary and material data. Desired features are:

- input simple data in simple way
- possibility to express very complex input data
- possibility to generate data automatically, and input very large input sets
- input interface that provides uniform access to the data in program independent of the input format

[... something else?]

As this is a draft version there are lot of remarks, suggestions and questions in square brackets. Some keys are marked OBSOLETE, which means that we want to replace them by something else.

3.1.1 CON file format

The root input file is in the Humanized JSON file format. That is the JSON file format with few syntax extensions and several semantic rules particular to Flow123d. The syntax extensions are

1. You can use one line comments using hash `#`.
2. The quoting of the keys is optional if they do not contain spaces (holds for all Flow keys).
3. You can use equality sign `=` instead of colon `:` for separation of keys and values in JSON objects.
4. You can use any whitespace to separate tokens in JSON object or JSON array.

The aim of these extensions is to simplify writing input files manually. However these extensions can be easily filtered out and converted to the generic JSON format. (This way it can be also implemented in Flow123d.)

For those who are not familiar with the JSON file format, we give the brief description right here. The full description can be found at http://www.json.org/. However, we use term *record* in the place of the *JSON object* in order to distinguish *JSON object*, which is merely a data structure written in the text, and the *C++ object*, i.e. instance of some class.

3.1.2 Humanized JSON

The JSON format consists of four kind of basic entities: *null* token, *true* and *false* tokens, *number*, *string*. *Number* is either integer or float point number possibly in the exponential form and *string* is any sequence of characters quoted in `""` (backslash `\` is used as escape character and Unicode is supported, see full specification for details).

In the following, we mean by white space characters: space, tab, and new line. In particular the newline character (outside of comment or quoting) is just the white space character without any special meaning.

The basic entities can be combined in composed entities, in a *record* or in an *array*. The *record* is set of assignments enclosed in the curly brackets

```
{
        #basic syntax
        "some_number":124,
        "some_string":"Hallo",
        "some_subrecord":{},
        "some_array":[],

        #extended syntax
        non_quoted_key_extension=123,
        separation_by_whitespace="a" sbw_1="b"
        sbw_2="c"
}
```

One assignment is a pair of the *key* and the *value*. *Key* is *string* or token matching regexp
`[a-zA-Z_][a-zA-Z_0-9]*`. *Value* is basic or composed entity. The key and the value are separated by the colon (generic syntax) or equality sign (extended syntax). Pairs are separated by a comma (generic syntax) or sequence of white space characters (extended syntax). The values stored in the record are accessed through the keys like in an associative array. Records are usually used for initialization of corresponding classes.

The second composed entity is the *array* which is sequence of (basic or composed) entities separated by comma (generic syntax) or whitespace sequence (extended syntax) and enclosed in the square brackets. The values stored in the array are accessed through the order. The Flow reader offers either initialization of a container from JSON array or a sequential access. The latter one is the only possible access for the included arrays, which we discuss later.

On any place out of the quoted string you can use hash mark `#` to start a one line comment. Everything up to the new line will be ignored and replaced by single white space.

[What about multiple line strings? (Should be allowed)]

3.1.3 CONSpecial keys

Apart from small extensions of JSON syntax, we impose further general rules on the interpretation of the input files by Flow123d reader. First, the capital only keywords have a special meaning for Flow JSON reader. On the other hand, we use only small caps for keys interpreted through the reader. The special keywords are:

TYPE :

```
TYPE= <enum>
```

The `<enum>` is particular semantic construct described later on. When appears in the record, it specifies which particular class to instantiate. This only has meaning if the record initializes an abstract class. In consistency with the source code, we shall call such records *polymorphic*.

In fact we consider that every record is of some *type* at least implicitly. The *type* of the record is specification of the keys that are interpreted by the program Flow123d. At some places the program assumes a record of specific *type* so you need not to specify `TYPE` key in those records.

INCLUDE_RECORD :

This is a simple inclusion of another file as a content of a record:

```
{
        INCLUDE_RECORD = "<file name>"
}
```

INCLUDE_ARRAY :

```
array=
{
        INCLUDE_ARRAY = "<file name>"
        FORMAT = "<format string>"
}
```

The reader will substitute the include record by a sequentially accessible array. The file has fixed number of space separated data fields on every line. Every line becomes one element in the array of type record. Every line forms a record with key names given by the `<format string>` and corresponding data taken form the line.

The key difference compared to regular JSON arrays is that included arrays can be accessed only sequentially within the program and thus we minimize reader memory overhead for large input data. The idea is to translate raw data into structured format and use uniform access to the data.

Basic syntax for format string could be an array of strings — formats of individual columns. Every format string is an address of key that is given the column. Onother possibility is to give an arbitrary JSON file, where all values are numbers of columns where to take the value.

[. . . better specify format string]

[Possible extensions: - have sections in the file for setting time dependent data - have number of lines at the beginning - have variable format - allow vectors in the 'line records']

REFERENCE :

```
time_governor={
  REF=<address>
}
```

This will set key `time_governor` to the same value as the entity specified by the address. The address is an array of strings for keys and integers for indices. The address can be absolute or relative identification of an entity. The relative address is relative to the entity in which the reference record is contained. One can use string `".."` to move to parent entity and string `"//"` to move to the root record of current file. Indices in address starts from 0.

For example assume the file

```
mesh={
        file_name="xyz"
}
array=[
        {x=1, y=0}
        {x=2, y=0}
        {x=3, y=0}
]
```

```
outer_record={
        output_file="x_out"
        inner_record={
                output_file={REF=["..","output_file"]}  # value "x_out"
        }
        x={REF="/array/2/x"}                                    # value "3"
        f_name={REF=["//","mesh","file_name"]}                  # value "xyz"
}
```

Concept of addres should be better explained and used consistently in reader interface.

3.1.4 Semantic rules

Implicit creation of composed entities

Consider that there is a *type* of record in which all keys have default values (possibly except one). Then the specification of the record *type* can contain a *default key*. Then user can use the value of the *default key* instead of the whole record. All other keys apart from the *default key* will be initialized by default values. This allows to express simple tasks by simple inputs but still make complex inputs possible. In order to make this working, developers should provide default values everywhere it is possible.

Similar functionality holds for arrays. If the user sets a non-array value where an array is expected the reader provides an array with a unique element holding the given value. See examples in the next section for application of these two rules.

Enum construct

Enum values can be integers or strings from particular set. Strings should be preferred for manual creating of input files, while the integer constants are suitable for automatic data preparation.

The input reader provides a way how to define names of members of an enum class and then initialize this enum class from input file. [Need better description]

String types

For purpose of this documentation we distinguish several string types with particular purpose and treatment. Those are:

input filename This has to be valid absolute or relative path to an existing file. The string can contain variable `${INPUT}` which will be replaced by path given at command line through parameter `-i`.

[In order to allow input of time dependent data in individual files, we should have also variable `${TIME\_LEVEL}` From user point of view this is not property of general input filename string, however in implementation this should be done in the same way as `${INPUT}`.]

[? Shall we allow both Windows and UNIX slashes?]

[Developers should provide default names to all files.]

output filename This has to be relative path. The path will be prefixed by the path given at command line through the parameter `-o`. In some cases the path will be also postfixed by extension of particular file format.

formula Expression that will be parsed and evaluated runtime. Documentation of particular key should provide variables which can appear in the expression, however in general it can be function of the space coordinates x, y, z and possibly also function of time t. For full specification of expression syntax see documentation of FParser library: http://warp.povusers.org/FunctionParser/fparser.html#literals

text string Just text without particular meaning.

Record types

A record type like particular definition of a class (e.g. in C++). One record type serves usually for initialization of one particular class. From this point of view one record type is set of keys that corresponding class can read.

For purpose of this manual the record type is given by specification of record's keys, their types, default values and meanings. In the next two sections, we describe all record types that forms input capabilities of Flow123d. Description of a record type has form of table. Table heading consists of the name of the record type. Then for every key we present name, type of the value, default value and text description of key meaning. Type of the value can be record type, array of record types, double, integer, enum or string type. Default value specification can be:

none No default value given, but input is mandatory. You get an error if you don't set this key.

null `null` value. No particular default value, but you need not to set the key. Usually means feature turned off.

explicit value For keys of type: string, double, integer, or enum, the default value is explicit value of this type.

type defaults For keys of some record type we let that record to set its default values.

[? polymorphic record types]

3.2 Record types for input of data fields

In this section we describe record types used to describe general time-space scalar, vector, or tensor fields and records for prescription of boundary conditions. Since one possibility how to prescribe input data fields is by discrete function spaces on computational mesh, we begin with mesh setting.

3.2.1 Mesh type

The mesh record and should provide a mesh consisting of points, lines, triangles and tetrahedrons in 3D space and further definition of boundary segments and element connectivity.

record type: **Mesh**

`file` = <*input filename*> DEFAULT: mesh.msh

The file with computational mesh in the ASCII GMSH format.
http://geuz.org/gmsh/doc/texinfo/gmsh.html#MSH-ASCII-file-format

`boundary_segments` = <*array of boundary segments*> DEFAULT: null optional

The set of 0,1, or 2 dimensional boundary faces of the mesh should be partitioned into boundary segments in order to prescribe unique boundary condition on every boundary face. The segments numbers are assigned to boundary faces by iterating through the array. Initially every boundary face has segment number 0. Every record in the array use "auxiliary" physical domains, elements or direct face specification to specify some set of boundary faces. The new segment number is assigned to each face in the set, possibly overwriting previous value.

Physical domains or its parts that appears in the boundary segment definitions are removed form the computational mesh, however, the element numbers of removed elements are stored in the corresponding boundary face and can be used to define face-wise approximations of functions with support on the boundary.

`neighbouring` = <*input file name*> DEFAULT: neigbours.flw

This should be removed as soon as we integrate ngh functionality into flow.

---

record type: **Boundary segment**

`index` = <*integer*> DEFAULT: index in outer array

The index of boundary segment can be used later to prescribe particular type of boundary condition on it. Indices must be greater or equal to 1 and should form more or less continuous sequence. The zero boundary segment is reserved for remaining part of the boundary. By default we assign indices to boundary segments according to the order in their array in mesh, i.e. index (counted form 0) plus 1.

`physical_domains` = <*array of integers*> DEFAULT: null optional

Numbers of physical domains which form the boundary segment. All elements of these physical domains will be removed from actual computational mesh.

`elements` = <*array of integers*> DEFAULT: null optional

The array contains element numbers which should be removed from computational mesh and added to boundary segment.

`sides` = <*array of integer pairs*> DEFAULT: null optional

The array contains numbers of elements which outer faces will be added to the boundary segment or pairs $[element, side\_on\ _{e}lement]$ identifying individual faces

that will be added to the boundary segment.

3.2.2 Time-space field type

A general time and space dependent, scalar, vector, or tensor valued function is given by array of *steady field data*, i.e. time slices. The time slice contains array of *space functions* for individual materials. Then, the *space function* can by either analytical (given by formula) or numerical, given by type of discrete space and array of *elemental functions*. *Elemental function* is just array of values for every degree of freedom on one element.

The function described by this type is tensor values in general and dimensions of this tensor should be specified outside of the function data. For example in description of Transport record type you should specify that function for initial condition is vector valued with vector size equal to number of substances. It is like template for Time-space field type parametrized by shape of the value tensor given by number of lines N and columnes N.

record type: **Steady field data**

`time` = <*double*> DEFAULT: -Inf

Start time for the spatial filed data.

`time_interpolation` = <*enum*> DEFAULT: constant

time interpolation enum cases:

`constant=0` Keeps constant data until next time cut.

`linear=1` Linear interpolation between current time cut and the next one.

`materials` = <*array of Steady spatial functions*> DEFAULT: null optional

record type: **Space function**

`material` = <*integer*> DEFAULT: 0

Material filter. The function has nonzero value only on elements with given material number. Function with filter 0 takes place for all materials where no function is set.

`analytic` = <*multi-array of function formulas*> DEFAULT: null optional

The shape of the multi-array is given by rank of the value of the function. Since formula parser can deal only with scalar functions, we have to specify individual members of resulting tensor. Formulas can contain variables x, y, z, and t. The formula is used until the next time slice and is evaluated for every solved time step (can depend on equation).

Instead of constant formulas one can use double values. Usage of formulas or doubles need not to be uniform over the tensor.

`numeric_type` = <*enum*> DEFAULT: None

FE space enum cases:

`None=0` Use analytic function.

`P0=1` Zero order polynomial on element.

Currently we support only P0 base functions for data.

`numeric` = <*array of element functions*> DEFAULT: empty array

Usually, this element-wise array should by included from an external file through `INCLUDE_ARRAY` construct.

---

record type: **Element function**

`element_id` = <*integer*> DEFAULT: null optional

Element ID in the mesh. By default the element is identified by the index in the array of element function.

`values` = <*multi-array of doubles*> DEFAULT: null mandatory

Values for degrees of freedom of the base functions on the element. Currently we support only P0 functions which are given by value in the barycenter of the element. In general the value can be tensor, i.e. array of arrays of doubles. However, in accordance to simplification rules, you can use only array of doubles for vector functions or mere double for scalar functions.

[tensor/vector valued element function should be given also as simple array of DOF values. But we have to provide ordering of tensor products of FE spaces]

[As follows from next examples, there is no way how to simply set simply tensors. We can introduce automatic conversion form scalar to vector (constant vector) and vector to tensor (diagonal tensor).]

[we should also allow 'in place' array includes to simplify material tables etc.]

[How to allow parallel input of field data?]

[Should be there explicit mesh reference in the field specification?]

Examples:

```
constant_scalar_function = 1.0
# is same as
constant_scalar_function = {
  time = -Inf,
  time_interpolation= constant,
  materials = [
    {
      rank=0
      numeric_type=None
      analytic=1.0       # the only key withou default value
    }
  ]
}

conductivity_tensor =
  [{ material = 1,
```

```
    rank = 2,
    analytic = [[1.0, 0.0, 0.0], [0.0, 1.0, 0.0], [0.0, 0.0, 1.0]]
  },
  { material = 2,
    rank = 2,
    analytic = [[10.0, 0.0, 0.0], [0.0, 10.0, 0.0], [0.0, 0.0, 10.0]]
  }
]
```

3.2.3 Boundary conditions

Input of boundary conditions is similar to the Time-space fields. For description of one time slice we have type *steady boundary data*. This contains array of *boundary conditions* for individual boundary segments. *Boundary condition* is given by type and parameters that are analytic or numeric functions. However, numeric functions are considered only on boundary elements.

record type: **steady boundary data**

`time` = <*double*> DEFAULT: 0.0

Time when the BC should be applied.

`bc` = <*array of boundary conditions*> DEFAULT: empty

record type: **boundary condition**

`boundary_segment` = <*integer*> DEFAULT: 0

Boundary segment where the boundary condition will be applied.

`bc_type` = <*enum*> DEFAULT: dirichlet

Currently there are just three types of boundary condition common to all equations, but some equations can implement some specific boundary conditions. Common boundary condition types are **BC types** enum cases:

`dirichlet=0`

`neumann=1`

`newton=2` (also known as Robin boundary condition)

`value` = <*space function*> DEFAULT: type defaults

Prescribed value for Dirichlet boundary condition and Newton boundary condition, the normal flux for the Neumann boundary condition. Key `material` of *space function* is irrelevant.

`mean_value` = <*scalar or vector constant*> DEFAULT: 0

Prescribes flux for Neumann boundary condition by total flux over the boundary segment. If both *value* and *mean_value* keys are set, we use only *value* key. [How this interact with fracture opening?]

`newton_coef` = <*scalar space function*> DEFAULT: type defaults

Coefficient that appears in the Newton boundary condition. Key `material` of *space function* is irrelevant.

E.g. denoting u the unknown scalar or vector field and $\partial_n u$ density of the normal flux of this field, the meaning of keys `value` and `newton_coef` is following: $\boldsymbol{v}\ \nabla v$

$u := value$	for Dirichlet boundary
$A\nabla u \cdot \boldsymbol{n} := value$	for Neumann boundary
$A\nabla u \cdot \boldsymbol{n} := newton_coef(u - value)$	for Newton boundary

Specific interpretation of the boundary conditions should be described in particular equations.

[How to allow both analytic and numerical functions here?]

[In order to allow changing BC type in time, the structure has to be: time array of BC segments array of BC type with data alternatively we can have just one array of BC patches, where one patch has: time, BC segment, BC type, BC data patches with non monotone time will be scratched]

[need vector valued Dirichlet (and Neuman, and Newton) for Transport boundary conditions]

[More examples...]

3.3 Other record types recognized by Flow123d

3.3.1 Record types not related to equations

record type: **Root record**

`system` = <*system type*> DEFAULT: type defaults

Record with application setting.

`problem` = <*problem type*> DEFAULT: null mandatory

Record with numerical problem to solve.

`material` = <*input filename*> DEFAULT: material.flw

Old material file still used for initialization of data fields in equations. This should be replaced by material database type. Then certain input data fields in equations can be constructed from material informations. Main obstacle are various adsorption algorithms depending on material number.

Only these keys are recognized directly at main level, however you can put here your own keys and then reference to them. For example `mesh` is part of problem type record, but you can put it on the main level and use reference inside `problem`.

[Should we put problem record to the main level?]

[Should we provide "material database"? Possibility to specify properties of individual materials and use them to construct field data for equations.]

record type: **System**

Description. lkajs eflakd flakds fropi pwnfvpweiurv evm qoiefmv lksdm vqoierrv lakfdsvkjweroivlksdmvaoirrf vm a v ve lkvqekfv jf ais i qkd ffo qk dfjhaopdif u wqwddff if j khr if

`pause_after_run` = <*bool*> DEFAULT: no

Wait for press of Enter after run. Good for Windows users, but dangerous for batch computations. Should be rather an command-line option.

`verbosity` = <*bool*> DEFAULT: no

Turns on/off more verbose mode.

`output_streams` = <*output stream*> DEFAULT: null optional

One or more output data streams. There are two predefined output streams:

vtk ascii stream:

```
{
  name="dafault_vtk_ascii"
  file="flow_output"
  type="vtk_ascii"
}
```

GMSH ascii stream:

```
{
  name="dafault_gmsh_ascii"
  file="flow_output"
  type="gmsh_ascii"
}
```

Possibly here could be variables for check-pointing, debugging, timers etc.

record type: **Output stream**

`name` = <*string*> DEFAULT: null mandatory

Name of the output stream. This is used to set output stream for individual output data.

`file` = <*output filename string*> DEFAULT: stream name

File name of the output file for the stream. The file name should be without extension, the correct extension will be appended according to the format type.

`format` = <*enum*> DEFAULT: vtk_ascii

output format enum cases:

`vtk_ascii=0`

`gmsh_ascii=1`

`precision` = <*integer*> DEFAULT: 8

Number of valid decadic digits to output floating point data into the ascii file formats.

`copy_file` = <*output filename string*> DEFAULT: null optional

Optionally one can set copy file to output data into to different file formats.

`copy_format` = <*enum*> DEFAULT: null optional

`copy_precision` = <*integer*> DEFAULT: 8

3.3.2 Equation related record types

Up to now there is only one problem type: `TYPE=sequential\_coupling`, but in near future we should introduce full coupling e.g. for density driven flow.

The *s*equential coupling problem has following keys:

record type: **Sequential coupling** implements *Problem type*

`description` = <*string*> DEFAULT: null optional

Short text description of solved problem. Now it is only reported on the screen, but could be written into output files or used somewhere else.

`mesh` = <*mesh type*> DEFAULT: type defaults

The computational mesh common for both coupled equations.

`time_governor` = <*time governor type*> DEFAULT: type defaults

Common time governor setting. [Future: allow different setting for each equation]

`primary_equation` = <*darcy flow type*> DEFAULT: type defaults

Independent equation.

`secondary_equation` = <*transport type*> DEFAULT: null optional

Equation with some data dependent on the primary equation.

---

record type: **Time governor**

`init_time` = <*double*> DEFAULT: 0.0

Time when an equation starts its simulation.

`time_step` = <*double*> DEFAULT: 1.0

Initial time step.

`end_time` = <*double*> DEFAULT: 1.0

End time for an equation.

This record type should initialize `TimeGovernor` class, but there are still questions about steady TimeGovernor and if we allow user setting for other parameters.

There are three subtypes *steady saturated MH*, *unsteady saturated MH*, *unsteady saturated LMH* The common keys are:

record type: **Darcy flow**(abstract type)

`TYPE` = <*enum*> DEFAULT:

There are three implementations of Darcy flow. Most keys are common but unsteady solvers accept some extra keys. **darcy flow type** enum cases:

`steady_MH=0`

`unsteady_LMH=1`

`unsteady_MH=2`

`sources` = <*time-space field*> DEFAULT: 0

Density of water sources. Scalar valued field (1x1 tensor).

`sources_file` = <*input file name*> DEFAULT: null optional

File with sources in old format. (OBSOLETE)

`source_formula` = <*space function*> DEFAULT: 0

Space function that prescribes water source.

`coef_tensor` = <*tensor steady field*> DEFAULT: 1.0

Conductivity 3x3 tensor. [Should be always 3x3 and then restricted on 2d and 1d fractures.]

`boundary_condition` = <*array of steady boundary data*> DEFAULT: null mandatory

New scheme for setting boundary conditions.

`boundary_file` = <*input file name*> DEFAULT: null mandatory

File with boundary conditions in old format. (OBSOLETE)

`solver` = <*solver type*> DEFAULT: type defaults

`n_schurs` = <*integer*> DEFAULT: 2

Number of Schur complements to make. Valid values are 0,1,2.

`output` = <*darcy flow output type*> DEFAULT: typ defaults

This is just sub record to separate output setting.

`initial` = <*steady data type*> DEFAULT: null mandatory

Initial condition. Scalar valued field (1x1 tensor). (for unsteady only)

`initial_file` = <*input file name*> DEFAULT: null mandatory

File with initial condition in old format. (OBSOLETE)

`storativity` = <*steady data type*> DEFAULT: null mandatory

Storativity coefficient. Scalar valued field (1x1 tensor). (for unsteady only)

record type: **Darcy flow output**

`save_step` = <*double*> DEFAULT: null optional

Time step between outputs.

`output_times` = <*array of doubles*> DEFAULT: null optional

Force output in prescribed times. Can be combined with regular otuptu given by `save_step`.

`velocity_p0` = <*output stream name*> DEFAULT: default_vtk_ascii

`pressure_p0` = <*output stream name*> DEFAULT: default_vtk_ascii

`pressure_p1` = <*output stream name*> DEFAULT: default_vtk_ascii

3.3.3 Solver type

record type: **Solver type** (abstract)

`TYPE` = <*enum*> DEFAULT: petsc

solver types enum cases:

`petsc=0` Use any PETSc solver for MPIAIJ matrices.

`bddc=1` Use BDDC solver (need not to work with every equation).

`accuracy` = <*double*> DEFAULT: solvers defaults

Absolute residual tolerance.

`max_it` = <*integer*> DEFAULT: 1000

Maximum number of outer iterations.

`parameters` = <*string*> DEFAULT: null optional

String with options for PETSc solvers.

`export_to_matlab` = <*bool*> DEFAULT: no

Save every solved system in matlab format. Useful for debugging and numerical experiments.

3.3.4 Transport type

record type: **Transport type**

`TYPE` = <*enum*> DEFAULT:

Two types are sofar possible. The second type is for advection-diffusion equation which needs implicit solver. **transport type** enum cases:

`TransportOperatorSplitting=0`

`AdvectionDiffusion_DG=1`

`sorption` = <*bool*> DEFAULT: no

`dual_porosity` = <*bool*> DEFAULT: no

`transport_reactions` = <*bool*> DEFAULT: no

What kind of reactions is this? Age of water?

`sigma` = <*double*> DEFAULT: 0

Coefficient of diffusive transfer through fractures.

`alpha_l` = <*double*> DEFAULT: 0

Longitudal dispersivity.

`alpha_t` = <*double*> DEFAULT: 0

Transversal dispersivity.

`d_m` = <*double*> DEFAULT: 1e-6

Molecular diffusivity.

`dg_penalty` = <*double*> DEFAULT: 0

Penalty parameter influencing the discontinuity of the solution.

`reactions` = <*reaction type*> DEFAULT: null optional

Currently only Semchem is supported. [Interface to Phreaq ...]

`decays` = <*array of decays*> DEFAULT: null optional

`substances` = <*array of strings*> DEFAULT: null mandatory

Names for transported substances. Number of substances is given implicitly by size of the array.

`initial` = <*steady data type*> DEFAULT: null mandatory

Vector valued initial condition for mobile phase of all species.

`initial_others` = <*steady data type*> DEFAULT: null optional

Tensor valued initial condition for immobile, mobile-sorbed, immobile-sorbed phases and all species. (3 x n_substances). [alternatively have separate key for each phase]

`initial_file` = <*input file name*> DEFAULT: null mandatory

File with initial condition in old format. (OBSOLETE)

`boundary_condition` = <*array of steady boundary data*> DEFAULT: null mandatory

New scheme for setting boundary conditions.

`boundary_file` = <*input file name*> DEFAULT: null mandatory

File with boundary condition in old format. (OBSOLETE) For time dependent boundary conditions, the filename is postfixed with number of time level.

`bc_times` = <*array of doubles*> DEFAULT: null optional

Times for changing boundary conditions. If you set this variable, you have to prepare a separate file with boundary conditions for every time in the list. Filenames for individual time level are formed from BC filename by appending underscore and three digits of time level number, e.g. `transport_bcd_000, transport_bcd_001, etc.` (OBSOLETE)

`output` = <*transport output*> DEFAULT: type defaults

---

record type: **Transport output**

`save_step` = <*double*> DEFAULT: null optional

Time step between outputs.

`output_times` = <*array of doubles*> DEFAULT: null optional

Force output in prescribed times. Can be combined with regular otuptu given by `save_step`.

`mobile_p0` = <*output stream name*> DEFAULT: default_vtk_ascii

`immobile_p0` = <*output stream name*> DEFAULT: default_vtk_ascii

`mobile_sorbed_p0` = <*output stream name*> DEFAULT: default_vtk_ascii

`immobile_sorbed_p0` = <*output stream name*> DEFAULT: default_vtk_ascii

`mobile_p1` = <*output stream name*> DEFAULT: default_vtk_ascii

`immobile_p1` = <*output stream name*> DEFAULT: default_vtk_ascii

`mobile_sorbed_p1` = <*output stream name*> DEFAULT: default_vtk_ascii

`immobile_sorbed_p1` = <*output stream name*> DEFAULT: default_vtk_ascii

record type: **Decay chain**

`substance_ids` = <*array of integers*> DEFAULT: empty

Sequence of N ids of transported substances defining isotopes contained in the decay chain under consideration.

`nr_of_children` = <*array of integers*> DEFAULT: either empty or filled up with ones

Number of children of each vertex (belonging to one of isotopes) in a simple graph describing considered decay chain. (NOT USED, YET.)

`indices_of_children` = <*array of integers*> DEFAULT: either emmpty or filled up with substanc

Containes identifiers of children of vertex. Children are assigned to vertices throuh the use of numbers listed in nr_of_children. (NOT USED, YET.)

`half_lives` = <*array of doubles*> DEFAULT: empty

This array containes $N-1$ half-lives belonging to isotopes contained in the array substance_ids. If there are no bifurcation key specified, the decay chain is linear $1 \to 2 \to 3$. If there is the bifurcation key, the decay chain is branched $1 \to 2, 1 \to 3$. (Temporary solution.)

`bifurcation` = <*array of double*> DEFAULT: null optional

It should have as many items as the array indices_of_children $(N-1)$. It defines relative part of parental contribution in the case of division of decay chain into more branches. (NOT USED, YET.)
Contains $N-1$ probabilities for individual branches of the bifurcation decay. (Temporary solution.) They should sum to one.

---

record type: **First order reactions**

`substance_ids` = <*array_of_integers*> DEFAULT: empty

Sequence of K ids describing a set of consequtive kinetic reactions of the first order. It is meant to enable simulation of $A \to B \to C \to ... \to Z$ set of reactions easily. (NOT USED, YET.)

`kinetic_constants` = <*array or doubles*> DEFAULT: filled up with 0.0s

Sequence of $K-1$ doubles defining kinetic constants of partial reactions from the set defined in substance_ids. (NOT USED, YET.)

`nr_of_children` = <*array of integer*> DEFAULT: filled up with 1.0s

Number of children of each vertex (belonging to one of species) in a simple graph describing considered first order reactions. (NOT USED, YET.)

`indices_of_children` = <*array of integers*> DEFAULT: either emmpty or filled up with substanc

Containes identifiers of children of vertex. Children are assigned to vertices throuh the use of numbers listed in nr_of_children. (NOT USED, YET.)

`bifurcation` = <*array of double*> DEFAULT: null optional

It should have as many items as the array indices_of_children $(K-1)$. It defines relative part of parental contribution in the case of division of first order reactions describing graph into more branches. (NOT USED, YET.)

`kinetic_konstant` = <*double*> DEFAULT: 0.0

Defines kinetic konstant which describes a simple reaction of the type $A \to B$.

`substance_ids` = <*array of integers*> DEFAULT: empty

Contains 2 identifiers of subsatnces (species) which are taking part in considered reaction.

---

record type: **Simple reactions**

`decay_chains` = <*array of Decay chains*> DEFAULT: empty

Sequence of records describing decay chains under consideration. (NOT USED, YET.)

`first_order_reactions` = <*array of first order reactions*> DEFAULT: empty

Sequence of records describing first order reactions under consideration. (NOT USED, YET.)

`pade_nominator_degree` = <*integer*> DEFAULT: 2

This number defines the degree of matrix polynomial appearing in nominator of Pade approximant of a matrix exponential.

`pade_denominator_degree` = <*integer*> DEFAULT: 2

This number defines the degree of matrix polynomial appearing in denominator of Pade approximant of a matrix exponential.

3.4 Other input files

3.4.1 Mesh file format version 2.0

The only supported format for the computational mesh is MSH ASCII format produced by the GMSH software. You can find its documentation on:

http://geuz.org/gmsh/doc/texinfo/gmsh.html#MSH-ASCII-file-format

Comments concerning Flow123d:

- Every inconsistency of the file stops the calculation. These are:
  - Existence of nodes with the same *node-number*.
  - Existence of elements with the same *elm-number*.
  - Reference to non-existing node.
  - Reference to non-existing material (see below).
  - Difference between *number-of-nodes* and actual number of lines in nodes' section.
  - Difference between *number-of-elements* and actual number of lines in elements' section.
- By default Flow123d assumes meshes with *number-of-tags* = 3.

tag1 is number of material (reference to `.MTR` file) in the element.

tag2 is number of geometry region in which the element lies.

tag3 is partition number (CURRENTLY NOT USED).

In accordance with specification of GMSH mesh format.

- Currently, line (*type* = 1), triangle (*type* = 2) and tetrahedron (*type* = 4) are the only supported types of elements. Existence of an element of different type stops the calculation.
- Wherever possible, we use the file extension `.MSH`. It is not required, but highly recomended.
- This file format can be used also for storing simple dicrete scalar or vector fields. We support output into this format (see Section 3.5)

3.4.2 Neighbouring file format, version 1.0

The file is divided in two sections, header and data. The extension `.NGH` is highly recomended for files of this type.

`$NeighbourFormat`
`1.0` *file-type* *data-size*
`$EndNeighbourFormat`
`$Neighbours`
number-of-neighbours
neighbour-number *type* <*type-specific-data*>
`...`
`$EndNeighbours`

where

file-type `int` — is equal 0 for the ASCII file format.

data-size `int` — the size of the floating point numbers used in the file. Usually *data-size* = sizeof(double).

number-of-neighbours `int` — Number of neighbouring defined in the file.

neighbour-number `int` — is the number (index) of the n-th neighbouring. These numbers do not have to be given in a consecutive (or even an ordered) way. Each number has to be given only onece, multiple definition are treated as inconsistency of the file and cause stopping the calculation.

type `int` — is type of the neighbouring.

<*type-specific-data*> — format of this list depends on the *type*.

Types of neighbouring and their specific data

type = `10` — "Edge with common nodes", i.e. sides of elements with common nodes. (Possible many elements)

type = `11` — "Edge with specified sides", i.e. sides of the edge are explicitly defined. (Possible many elements)

type = `20` — "Compatible", i.e. volume of an element with a side of another element. (Only two elements)

type = `30` — "Non-compatible" i.e. volume od an element with volume of another element. (Only two elements)

type	*type-specific-data*	Description
10	*n_elm eid1 eid2 ...*	number of elements and their ids
11	*n_sid eid1 sid1 eid2 sid2 ...*	number of sides, their elements and local ids
20	*eid1 eid2 sid2 coef*	Elm 1 has to have lower dimension
30	*eid1 eid2 coef*	Elm 1 has to have lower dimension

coef is of the `double` type, other variables are `int`s.

Comments concerning `Flow123d`:

- Every inconsistency or error in the `.NGH` file causes stopping the calculation. These are especially:
  - Multiple usage of the same *neighbour-number*.
  - Difference between *number-of-neighbours* and actual number of data lines.
  - Reference to nonexisting element.
  - Nonsence number of side.
- The variables *sid?* must be nonegative and lower than the number of sides of the particular element.

3.4.3 Material properties file format, version 1.0

The file is divided in two sections, header and data. The extension `.MTR` is highly recomended for files of this type.

```
$MaterialFormat
1.0 file-type  data-size
$EndMaterialFormat
$Materials
number-of-materials
material-number  material-type <material-type-specific-data>  [text]
...
$EndMaterials
```

`$Storativity`
material-number <storativity-coefficient> [text]
...
`$EndStorativity`
`$Geometry`
material-number geometry-type <geometry-type-specific-coefficient> [text]
...
`$EndGeometry`
`$Sorption`
material-number substance-id sorption-type <sorption-type-specific-data> [text]
...
`$EndSorption`
`$SorptionFraction`
material-number <sorption-fraction-coefficient> [text]
...
`$EndSorptionFraction`
`$DualPorosity`
material-number <mobile-porosity-coefficient> <immobile-porosity-coefficient>
<nonequillibrium-coefficient-substance(0)>
...<nonequilibrium-coefficient-substance(n-1)> [text]
...
`$EndDualPorosity`
`$Reactions`
reaction-type <reaction-type-specific-coefficient> [text]
...
`$EndReactions`

where:

file-type `int` — is equal 0 for the ASCII file format.

data-size `int` — the size of the floating point numbers used in the file. Usually *data-size* = sizeof(double).

number-of-materials `int` — Number of materials defined in the file.

material-number `int` — is the number (index) of the n-th material. These numbers do not have to be given in a consecutive (or even an ordered) way. Each number has to be given only onece, multiple definition are treated as inconsistency of the file and cause stopping the calculation (exception $Sorption section).

material-type `int` — is type of the material, see table.

<material-type-specific-data > — format of this list depends on the *material - type*.

<storativity-coefficient> `double` — coefficient of storativity

geometry-type `int` — type of complement dimension parameter (only for 1D and 2D material), for 1D element is supported type 1 - cross-section area, for 2D element is supported type 2 - thickness.

<*geometry-type-specific-coefficient*> `double` — cross-section for 1D element or thickness for 2D element.

substance-id `int` — refers to number of transported substance, numbering starts on *0*.

sorption-type `int` — type 1 - linear sorption isotherm, type 2 - Freundlich sorption isotherm, type 3 - Langmuir sorption isotherm.

<*sorption-type-specific-data* > — format of this list depends on the *sorption - type*, see table.

Note: Section $Sorption is needed for calculation only if *Sorption* is turned on in the *ini* file.

<*sorption-fraction-coefficient*> `double` — ratio of the "mobile" solid surface in the contact with "mobile" water to the total solid surface (this parameter (section) is needed for calculation only if *Dual_porosity* and *Sorption* is together turned on in the ini file).

<*mobile-porosity-coefficient*> `double` — ratio of the mobile pore volume to the total volume (this parameter is needed only if *Transport_on* is turned on in the ini file).

<*immobile-porosity-coefficient*> `double` — ratio of the immobile pore volu-me to the total pore volume (this parameter is needed only if *Dual_porosity* is turned on in the ini file).

<*nonequilibrium-coefficient-substance(i)*> `double` — nonequilibrium coefficient for substance i, $\forall i \in \langle 0, n-1 \rangle$ where n is number of transported substances (this parameter is needed only if *Dual_porosity* is turned on in the ini file).

reaction-type `int` — type 0 - zero order reaction

<*reaction-type-specific-data* > — format of this list depends on the *reaction - type*, see table.

material-type	*material-type-specific-data*	Description
11	k	$\mathbf{K} = (k)$
-11	a	$\mathbf{A} = \mathbf{K}^{-1} = (a)$
21	k	$\mathbf{K} = \begin{pmatrix} k & 0 \\ 0 & k \end{pmatrix}$
22	$k_x \quad k_y$	$\mathbf{K} = \begin{pmatrix} k_x & 0 \\ 0 & k_y \end{pmatrix}$
23	$k_x \quad k_y \quad k_{xy}$	$\mathbf{K} = \begin{pmatrix} k_x & k_{xy} \\ k_{xy} & k_y \end{pmatrix}$
-21	a	$\mathbf{A} = \mathbf{K}^{-1} = \begin{pmatrix} a & 0 \\ 0 & a \end{pmatrix}$
-22	$a_x \quad a_y$	$\mathbf{A} = \mathbf{K}^{-1} = \begin{pmatrix} a_x & 0 \\ 0 & a_y \end{pmatrix}$
-23	$a_x \quad a_y \quad a_{xy}$	$\mathbf{A} = \mathbf{K}^{-1} = \begin{pmatrix} a_x & a_{xy} \\ a_{xy} & a_y \end{pmatrix}$
31	k	$\mathbf{K} = \begin{pmatrix} k & 0 & 0 \\ 0 & k & 0 \\ 0 & 0 & k \end{pmatrix}$
33	$k_x \quad k_y \quad k_z$	$\mathbf{K} = \begin{pmatrix} k_x & 0 & 0 \\ 0 & k_y & 0 \\ 0 & 0 & k_z \end{pmatrix}$
36	$k_x \quad k_y \quad k_z \quad k_{xy} \quad k_{xz} \quad k_{yz}$	$\mathbf{K} = \begin{pmatrix} k_x & k_{xy} & k_{xz} \\ k_{xy} & k_y & k_{yz} \\ k_{xz} & k_{yz} & k_z \end{pmatrix}$
-31	a	$\mathbf{A} = \mathbf{K}^{-1} = \begin{pmatrix} a & 0 & 0 \\ 0 & a & 0 \\ 0 & 0 & a \end{pmatrix}$
-33	$a_x \quad a_y \quad a_z$	$\mathbf{A} = \mathbf{K}^{-1} = \begin{pmatrix} a_x & 0 & 0 \\ 0 & a_y & 0 \\ 0 & 0 & a_z \end{pmatrix}$
-36	$a_x \quad a_y \quad a_z \quad a_{xy} \quad a_{xz} \quad a_{yz}$	$\mathbf{A} = \mathbf{K}^{-1} = \begin{pmatrix} a_x & a_{xy} & a_{xz} \\ a_{xy} & a_y & a_{yz} \\ a_{xz} & a_{yz} & a_z \end{pmatrix}$

Note: all variables (k, k_x, k_y, k_z, k_{xy}, k_{xz}, k_{yz}, a, a_x, a_y, a_z, a_{xy}, a_{xz}, a_{yz}) are of the `double` type.

sorption-type	*sorption-type-specific-data*	Description
1	$k_D[1]$	$s = k_D c$
2	$k_F[(L^{-3} \cdot M^1)^{(1-\alpha)}] \quad \alpha[1]$	$s = k_F c^\alpha$
3	$K_L[L^3 \cdot M^{-1}] \quad s^{max}[L^{-3} \cdot M^1]$	$s = \frac{K_L s^{max}\ c}{1+K_L c}$

Note: all variables (k_D, k_F, α, K_L, s^{max}) are of the `double` type.

reaction-type	*reaction-type-specific-data*	Description
0	*substance-id*[1] $\quad k[M \cdot L^{-3} \cdot T^{-1}]$	$\frac{\partial c_m^{[substance\text{-}id]}}{\partial t} = k$

Where $c_m^{[substance\text{-}id]}$ is mobile concentration of substance with id *substance-id* and Δt is the internal transport time step defined by CFL condition.

text `char[]` — is a text description of the material, up to 256 chars. This parameter is

optional.

Comments concerning `Flow123d`:

- If *number-of-materials* differs from actual number of material lines in the file, it stops the calculation.

3.4.4 Boundary conditions file format, version 1.0

The file is divided in two sections, header and data.

`$BoundaryFormat`
`1.0` *file-type data-size*
`$EndBoundaryFormat`
`$BoundaryConditions`
number-of-conditions
condition-number type <*type-specific-data*> *where* <*where-data*> *number-of-tags* <*tags*> *[text]*
`...`
`$EndBoundaryConditions`

where

file-type `int` — is equal 0 for the ASCII file format.

data-size `int` — the size of the floating point numbers used in the file. Usually *data-size* = sizeof(double).

number-of-conditions `int` — Number of boundary conditions defined in the file.

condition-number `int` — is the number (index) of the n-th boundary condition. These numbers do not have to be given in a consecutive (or even an ordered) way. Each number has to be given only onece, multiple definition are treated as inconsistency of the file and cause stopping the calculation.

type `int` — is type of the boundary condition. See below for definitions of the types.

<*type-specific-data*> — format of this list depends on the *type*. See below for specification of the *type-specific-data* for particular types of the boundary conditions.

where `int` — defines the way, how the place for the contidion is prescribed. See below for details.

<*where-data*> — format of this list depends on *where* and actually defines the place for the condition. See below for details.

number-of-tags `int` — number of integer tags of the boundary condition. It can be zero.

< *tags* > *number-of-tags*`*int` — list of tags of the boundary condition. Values are separated by spaces or tabs. By default we set *number-of-tags*=1, where *tag1* defines group of boundary conditions, "type of water" in our jargon. This can be used to calculate total fluxes through the boundary group.

[text] `char[]` — arbitrary text, description of the fracture, notes, etc., up to 256 chars. This is an optional parameter.

Types of boundary conditions and their data

type = `1` — Boundary condition of the Dirichlet's type

type = `2` — Boundary condition of the Neumann's type

type = `3` — Boundary condition of the Newton's type

type	*type-specific-data*	Description
1	*scalar*	Prescribed value of pressure (in meters [m])
2	*flux*	Prescribed value of flux through the boundary
3	*scalar sigma*	Scalar value and the σ coefficient

scalar, *flux* and *sigma* are of the `double` type.

Ways of defining the place for the boundary condition

where = `1` — Condition on a node

where = `2` — Condition on a (generalized) side

where = `3` — Condition on side for element with only one external side.

where	<*where-data*>	Description
1	*node-id*	Node id number, according to `.MSH` file
2	*elm-id sid-id*	Elm. id number, local number of side
3	*elm-id*	Elm. id number

The variables *node-id*, *elm-id*, *sid-id* are of the `int` type.

Comments concerning `Flow123d`:

- We assume homegemous Neumman's condition as the default one. Therefore we do not need to prescribe conditions on the whole boundary.
- If the condition is given on the inner edge, it is treated as an error and stops calculation.
- Any inconsistence in the file stops calculation. (Bad number of conditions, multiple definition of condition, reference to non-existing node, etc.)

- At least one of the conditions has to be of the Dirichlet's or Newton's type. This is well-known fact from the theory of the PDE's.
- Local numbers of sides for *where* = 2 must be lower than the number of sides of the particular element and greater then or equal to zero.
- The element specified for *where* = 3 must have only one external side, otherwise the program stops.

3.4.5 Transport boundary conditions file format, version 1.0

The file is divided in two sections, header and data.

`$Transport_BCDFormat`
`1.0` *file-type data-size*
`$EndTransport_BCDFormat`
`$Transport_BCD`
number-of-conditions
transport-condition-number boundary-condition-number value1 value2 ...
`$EndTransport_BCD`

where

file-type `int` - is equal 0 for the ASCII file format.

data-size `int` - the size of the floating point numbers used in the file. Usually data-size = sizeof(double)

number-of-conditions `int` - Number of conditions defined in the file.

transport-condition-number `int` - is the number (index) of the n-th transport condition. These numbers do not have to be given in a consecutive (or even an ordered) way. Each number has to be given only once, multiple definition are treated as inconsistency of the file and cause stopping the calculation.

boundary-condition-number `int` - id number of the boundary-condition where transport boundary condition is prescribed.

valueN `double` - prescribed boundary concentration of substance N (should be from interval $[0, 1]$).

Comments concerning FLOW123d: Number of transport boundary conditions has to be same as number of boundary conditions. Program stops computation in the other case.

3.4.6 Element data file format, version 1.0

Several input data fields are given as constant scalars on every element. In particular this is used for water sources, initial condition of pressure, initial condition for concentrations and substance sources in transport. Common file format of these files is:

```
$FieldName
number-of-lines
eid value1 value2 ...
...
$EndFieldName
```

where

`$FieldName` — Unique name of the input field. Since all field data are enclosed by `$FieldName` and `$EndFieldName` one can even have different fields in one common file.

number-of-sources `int` — Number of data lines that has to match number of elements in the mesh.

eid `int` — is id-number of the element (in the input mesh file).

valueN `double` — list of field values. Number of values is specific for each particular type of input.

Description of individual input fields.

water sources FieldName=`Sources`, there is only one value per line — the density of water source on the element.

pressure initial condition FieldName=`PressureHead`, there is only one value per line — the initial pressure value on the element.

substance sources FieldName=`TransportSources`, number of values is 3 times number of substances. The density of one substance source is given by formula:

$$f = d + \sigma(c - c_N)$$

where f is total source, the first term is fixed Neuman-like source density d. The second term is Newton-like source density, where σ is transmisitvity, c is actual concentration, and c_N is prescribed concentration. For every substance there is triplet of three parameters: d, σ, c_N. The order of substances is same as in the main INI file.

concentration initial conditions FieldName=`Concentrations`, number of values equal to number of transported substances, the order of substances is same as in the main INI file.

Comments concerning `Flow123d`:

- Every inconsistency or error in the `.SRC` file causes stopping the calculation. These are especially:
  - Difference between *number-of-lines* and actual number of data lines.
  - Reference to nonexisting element.

3.5 Output files

Flow123d support output of scalar and vaector data fields into two formats. First one can use native fromat of program GMSH (usualy with extension `msh`) which contains computational mesh and then various datafields for squence of time levels. For second we support output into XML version of VTK files. These files can be viewed and postprocessed by several vizualization softwares. However, our primal goal is to support data transfer into Paraview vizualization software. See key Pos_format.

3.5.1 Output data fields of water flow module

Water flow module provides output of four data fields.

pressure on elements Pressure head in length units $[L]$ piecewise constant on every element. This field is directly produced by the MH method and thus contains no postprocessing error.

pressure in nodes Same pressure head field, but interpolated into $P1$ continuous scalar field. Namely you lost dicontinuities on fractures.

velocity on elements Vector field of water flux volume unit per time unit $[L^3/T]$. For every element we evaluate discrete flux field in barycenter.

piezometric head on elements Piezometric head in length units $[L]$ piecewise constant on every element. This is just pressure on element plus z-coordinate of the barycenter. This field is produced only on demand (see key output_piezo_head).

3.5.2 Output data fields of transport

Transport module provides output only for concentrations (in mobile phase) as a field piecewise constant over elements. There is one field for every substance and names of those fields contain names of substances given by key Substances. The physical unit is mass unit over volume unit $[M/L^3]$.

3.5.3 Auxiliary output files

Profiling information

On every run we collect some bacis profilling informations. After all computations these data are written into the file `profiler%y%m%d_%H.%M.%S.out` where `%y`, `%m`, `%d`, `%H`, `%M`, `%S` are two digit numbers representing year, month, day, hour, minute, and second of the program start time.

Water flux information

File contains water flow balance, total inflow and outflow over boundary segments. Further there is total water income due to sources (if they are present).

Raw water flow data file

You can force Flow123d to write raw data about results of MH method. The file format is:

```
$FlowField
T=<time>
<number fo elements>
<eid> <pressure> <flux x> <flux y> <flux z> <number of sides> <pressures on sides> <flu
...
$EndFlowField
```

where

`<time>` — is simulation time of the raw output.

`<number of elements>` — is number of elements in mesh, which is same as number of subsequent lines.

`<eid>` — element id same as in the input mesh.

`<flux x,y,z>` — components of water flux interpolated to barycenter of the element

`<number of sides>` — number of sides of the element, infulence number of remaining values

`<pressures on sides>` — for every side average of the pressure over the side

`<fluxes on sides>` — for ever side total flux through the side

Chapter 4

Main input file reference

---

abstract type: **Problem**

Descendants:

The root record of description of particular the problem to solve.

SequentialCoupling

---

record: **SequentialCoupling** implements abstract type: Problem

---

Record with data for a general sequential coupling.

`TYPE` = *<selection: Problem_TYPE_selection>*

Default: SequentialCoupling []

Sub-record selection.

`description` = *<String (generic)>*

Default: *<optional>* []

Short description of the solved problem. Is displayed in the main log, and possibly in other text output files.

`mesh` = *<record: Mesh>*

Default: *<obligatory>* []

Computational mesh common to all equations.

`time` = *<record: TimeGovernor>*

Default: *<optional>* []

Simulation time frame and time step.

`primary_equation` = *<abstract type: DarcyFlowMH>*

Default: *<obligatory>* []

Primary equation, have all data given.

`secondary_equation` = *<abstract type: Transport>*

Default: *<optional>* []

The equation that depends (the velocity field) on the result of the primary equation.

---

record: **Mesh**

Record with mesh related data.

`mesh_file` = *<input file name>*

Default: *<obligatory>* []

Input file with mesh description.

`regions` = *<Array of record: Region>*

Default: *<optional>* []

List of additional region definitions not contained in the mesh.

`sets` = *<Array of record: RegionSet>*

Default: *<optional>* []

List of region set definitions. There are three region sets implicitly defined: ALL (all regions of the mesh), BOUNDARY (all boundary regions), and BULK (all bulk regions)

---

record: **Region**

Definition of region of elements.

`name` = *<String (generic)>*

Default: *<obligatory>* []

Label (name) of the region. Has to be unique in one mesh.

`id` = *<Integer [0,]>*

Default: *<obligatory>* []

The ID of the region to which you assign label.

`element_list` = *<Array of Integer [0,]>*

Default: *<optional>* []

Specification of the region by the list of elements. This is not recomended

---

record: **RegionSet**

Definition of one region set.

`name` = *<String (generic)>*

Default: *<obligatory>* []

Unique name of the region set.

`region_ids` = *<Array of Integer [0,]>*

Default: <*optional*> []

List of region ID numbers that has to be added to the region set.

`region_labels` = <*Array of String (generic)*>

Default: <*optional*> []

List of labels of the regions that has to be added to the region set.

`union` = <*Array [2, 2] of String (generic)*>

Default: <*optional*> []

Defines region set as a union of given pair of sets. Overrides previous keys.

`intersection` = <*Array [2, 2] of String (generic)*>

Default: <*optional*> []

Defines region set as an intersection of given pair of sets. Overrides previous keys.

`difference` = <*Array [2, 2] of String (generic)*>

Default: <*optional*> []

Defines region set as a difference of given pair of sets. Overrides previous keys.

---

record: **TimeGovernor**

Setting of the simulation time. (can be specific to one eqaution)

`start_time` = <*Double* >

Default: 0.0 []

Start time of the simulation.

`end_time` = <*Double* >

Default: <*obligatory*> []

End time of the simulation.

`init_dt` = <*Double [0,]*>

Default: <*optional*> []

Initial guess for the time step. The time step is fixed if hard time step limits are not set.

`min_dt` = <*Double [0,]*>

Default: "Machine precision or 'init_dt' if specified" []

Hard lower limit for the time step.

`max_dt` = <*Double [0,]*>

Default: "Whole time of the simulation or 'init_dt' if specified" []

Hard upper limit for the time step.

---

abstract type: **DarcyFlowMH**

Descendants:

Mixed-Hybrid solver for saturated Darcy flow.

Steady_MH

Unsteady_MH

Unsteady_LMH

record: **Steady_MH** implements abstract type: DarcyFlowMH

Mixed-Hybrid solver for STEADY saturated Darcy flow.

`TYPE` = *<selection: DarcyFlowMH_TYPE_selection>*

Default: Steady_MH []

Sub-record selection.

`n_schurs` = *<Integer [0, 2]>*

Default: 2 []

Number of Schur complements to perform when solving MH sytem.

`solver` = *<abstract type: Solver>*

Default: *<obligatory>* []

Linear solver for MH problem.

`output` = *<record: DarcyMHOutput>*

Default: *<obligatory>* []

Parameters of output form MH module.

`mortar_method` = *<selection: MH_MortarMethod>*

Default: None []

Method for coupling Darcy flow between dimensions.

`mortar_sigma` = *<Double [0,]>*

Default: 1.0 []

Conductivity between dimensions.

`bc_data` = *<Array of record: DarcyFlowMH_Steady_BoundaryData>*

Default: *<obligatory>* []

`bulk_data` = *<Array of record: DarcyFlowMH_Steady_BulkData>*

Default: *<obligatory>* []

abstract type: **Solver**

Descendants:

Solver setting.

Petsc

Bddc

---

record: **Petsc** implements abstract type: Solver

Solver setting.

`TYPE` = *<selection: Solver_TYPE_selection>*

Default: Petsc []

Sub-record selection.

`a_tol` = *<Double [0,]>*

Default: 1.0e-9 []

Absolute residual tolerance.

`r_tol` = *<Double [0, 1]>*

Default: 1.0e-7 []

Relative residual tolerance (to initial error).

`max_it` = *<Integer [0,]>*

Default: 10000 []

Maximum number of outer iterations of the linear solver.

`options` = *<String (generic)>*

Default: []

Options passed to the petsc instead of default setting.

---

record: **Bddc** implements abstract type: Solver

Solver setting.

`TYPE` = *<selection: Solver_TYPE_selection>*

Default: Bddc []

Sub-record selection.

`a_tol` = *<Double [0,]>*

Default: 1.0e-9 []

Absolute residual tolerance.

`r_tol` = *<Double [0, 1]>*

Default: 1.0e-7 []

Relative residual tolerance (to initial error).

`max_it` = *<Integer [0,]>*

Default: 10000 []

Maximum number of outer iterations of the linear solver.

record: **DarcyMHOutput**

Parameters of MH output.

`save_step` = <*Double [0,]*>

Default: 1.0 []

Regular step between MH outputs.

`output_stream` = <*record: OutputStrem*>

Default: <*obligatory*> []

Parameters of output stream.

`velocity_p0` = <*String (generic)*>

Default: <*optional*> []

Output stream for P0 approximation of the velocity field.

`pressure_p0` = <*String (generic)*>

Default: <*optional*> []

Output stream for P0 approximation of the pressure field.

`pressure_p1` = <*String (generic)*>

Default: <*optional*> []

Output stream for P1 approximation of the pressure field.

`piezo_head_p0` = <*String (generic)*>

Default: <*optional*> []

Output stream for P0 approximation of the piezometric head field.

`balance_output` = <*output file name*>

Default: water_balance.txt []

Output file for water balance table.

`raw_flow_output` = <*output file name*>

Default: <*optional*> []

Output file with raw data form MH module.

record: **OutputStrem**

Parameters of output.

`name` = <*String (generic)*>

Default: <*obligatory*> []

The name of this stream. Used to reference the output stream.

`file` = <*output file name*>

Default: <*obligatory*> []

File path to the output stream.

`format` = <*abstract type: OutputFormat*>

Default: <*optional*> []

Format of output stream and possible parameters.

---

abstract type: **OutputFormat**

Descendants:

Format of output stream and possible parameters.

vtk

gmsh

---

record: **vtk** implements abstract type: OutputFormat

Parameters of vtk output format.

`TYPE` = <*selection: OutputFormat_TYPE_selection*>

Default: vtk []

Sub-record selection.

`variant` = <*selection: VTK variant (ascii or binary)*>

Default: ascii []

Variant of output stream file format.

`parallel` = <*Bool*>

Default: false []

Parallel or serial version of file format.

`compression` = <*selection: Type of compression of VTK file format*>

Default: none []

Compression used in output stream file format.

---

selection type: **VTK variant (ascii or binary)**

Possible values:

`ascii` : ASCII variant of VTK file format

`binary` : Binary variant of VTK file format (not supported yet)

---

selection type: **Type of compression of VTK file format**

Possible values:

`none` : Data in VTK file format are not compressed

`zlib` : Data in VTK file format are compressed using zlib (not supported yet)

record: **gmsh** implements abstract type: OutputFormat

Parameters of gmsh output format.

`TYPE` = <*selection: OutputFormat_TYPE_selection*>

Default: gmsh []

Sub-record selection.

selection type: **MH_MortarMethod**

Possible values:

`None` : Mortar space: P0 on elements of lower dimension.

`P0` : Mortar space: P0 on elements of lower dimension.

`P1` : Mortar space: P1 on intersections, using non-conforming pressures.

record: **DarcyFlowMH_Steady_BoundaryData**

Record to set BOUNDARY fields of the equation 'DarcyFlowMH_Steady'. The fields are set only on the domain specified by one of the keys: 'region', 'rid', 'r_set' and after the time given by the key 'time'. The field setting can be overridden by any DarcyFlowMH_Steady_BoundaryData record that comes later in the boundary data array.

`r_set` = <*String (generic)*>

Default: <*optional*> []

Name of region set where to set fields.

`region` = <*String (generic)*>

Default: <*optional*> []

Label of the region where to set fields.

`rid` = <*Integer [0,]*>

Default: <*optional*> []

ID of the region where to set fields.

`time` = <*Double [0,]*>

Default: 0.0 []

Apply field setting in this record after this time. These times has to form an increasing sequence.

`bc_type` = <*abstract type: Field:R3 → Enum*>

Default: <*optional*> []

Boundary condition type, possible values:

`bc_pressure` = <*abstract type: Field:R3 → Real*>

Default: <*optional*> []

Dirichlet BC condition value for pressure.

`bc_flux` = <*abstract type: Field:R3 → Real*>

Default: <*optional*> []

Flux in Neumman or Robin boundary condition.

`bc_robin_sigma` = <*abstract type: Field:R3 → Real*>

Default: <*optional*> []

Conductivity coefficient in Robin boundary condition.

`bc_piezo_head` = <*abstract type: Field:R3 → Real*>

Default: <*optional*> []

Boundary condition for pressure as piezometric head.

`flow_old_bcd_file` = <*input file name*>

Default: <*optional*> []

---

abstract type: **Field:R3 → Enum** default descendant: FieldConstant

---

Descendants:

Abstract record for all time-space functions.

`FieldConstant`

`FieldFormula`

`FieldPython`

`FieldElementwise`

---

record: **FieldConstant** implements abstract type: Field:R3 → Enum constructible from key: value

---

R3 → Enum Field constant in space.

`TYPE` = <*selection: Field:R3 → Enum_TYPE_selection*>

Default: FieldConstant []

Sub-record selection.

`value` = <*selection: EqData_bc_Type*>

Default: <*obligatory*> []

Value of the constant field. For vector values, you can use scalar value to enter constant vector. For square NxN-matrix values, you can use: * vector of size N to enter diagonal matrix * vector of size (N+1)*N/2 to enter symmetric matrix (upper triangle, row by row) * scalar to enter multiple of the unit matrix.

---

selection type: **EqData_bc_Type**

Possible values:

`none` : Homogeneous Neoumann BC.

`dirichlet` :

`neumann` :

`robin` :

`total_flux` :

---

record: **FieldFormula** implements abstract type: Field:R3 → Enum

---

R3 → Enum Field given by runtime interpreted formula.

`TYPE` = *<selection: Field:R3 → Enum_TYPE_selection>*

Default: FieldFormula []

Sub-record selection.

`value` = *<String (generic)>*

Default: *<obligatory>* []

String, array of strings, or matrix of strings with formulas for individual entries of scalar, vector, or tensor value respectively. For vector values, you can use just one string to enter homogeneous vector. For square NxN-matrix values, you can use: * array of strings of size N to enter diagonal matrix * array of strings of size (N+1)*N/2 to enter symmetric matrix (upper triangle, row by row) * just one string to enter (spatially variable) multiple of the unit matrix. Formula can contain variables x,y,z,t and usual operators and functions.

---

record: **FieldPython** implements abstract type: Field:R3 → Enum

---

R3 → Enum Field given by a Python script.

`TYPE` = *<selection: Field:R3 → Enum_TYPE_selection>*

Default: FieldPython []

Sub-record selection.

`script_string` = *<String (generic)>*

Default: "Obligatory if 'script_file' is not given." []

Python script given as in place string

`script_file` = *<input file name>*

Default: "Obligatory if 'script_striong' is not given." []

Python script given as external file

`function` = *<String (generic)>*

Default: *<obligatory>* []

Function in the given script that returns tuple containing components of the return type. For NxM tensor values: tensor(row,col) = tuple(M*row + col).

---

record: **FieldElementwise** implements abstract type: Field:R3 → Enum

R3 → Enum Field constant in space.

`TYPE` = <*selection: Field:R3 → Enum_TYPE_selection*>

Default: FieldElementwise []

Sub-record selection.

`gmsh_file` = <*input file name*>

Default: <*obligatory*> []

Input file with ASCII GMSH file format.

`field_name` = <*String (generic)*>

Default: <*obligatory*> []

The values of the Field are read from the $ElementData section with field name given by this key.

---

abstract type: **Field:R3 → Real** default descendant: FieldConstant

Descendants:

Abstract record for all time-space functions.

`FieldConstant`

`FieldPython`

`FieldFormula`

`FieldElementwise`

`FieldInterpolatedP0`

---

record: **FieldConstant** implements abstract type: Field:R3 → Real constructible from key: value

R3 → Real Field constant in space.

`TYPE` = <*selection: Field:R3 → Real_TYPE_selection*>

Default: FieldConstant []

Sub-record selection.

`value` = <*Double* >

Default: <*obligatory*> []

Value of the constant field. For vector values, you can use scalar value to enter constant vector. For square NxN-matrix values, you can use: * vector of size N to enter diagonal matrix * vector of size (N+1)*N/2 to enter symmetric matrix (upper triangle, row by row) * scalar to enter multiple of the unit matrix.

---

record: **FieldPython** implements abstract type: Field:R3 → Real

R3 → Real Field given by a Python script.

`TYPE` = <*selection: Field:R3 → Real_TYPE_selection*>

Default: FieldPython []

Sub-record selection.

`script_string` = <*String (generic)*>

Default: "Obligatory if 'script_file' is not given." []

Python script given as in place string

`script_file` = <*input file name*>

Default: "Obligatory if 'script_striong' is not given." []

Python script given as external file

`function` = <*String (generic)*>

Default: <*obligatory*> []

Function in the given script that returns tuple containing components of the return type. For NxM tensor values: tensor(row,col) = tuple(M*row + col).

---

record: **FieldFormula** implements abstract type: Field:R3 → Real

---

R3 → Real Field given by runtime interpreted formula.

`TYPE` = <*selection: Field:R3 → Real_TYPE_selection*>

Default: FieldFormula []

Sub-record selection.

`value` = <*String (generic)*>

Default: <*obligatory*> []

String, array of strings, or matrix of strings with formulas for individual entries of scalar, vector, or tensor value respectively. For vector values, you can use just one string to enter homogeneous vector. For square NxN-matrix values, you can use: * array of strings of size N to enter diagonal matrix * array of strings of size (N+1)*N/2 to enter symmetric matrix (upper triangle, row by row) * just one string to enter (spatially variable) multiple of the unit matrix. Formula can contain variables x,y,z,t and usual operators and functions.

---

record: **FieldElementwise** implements abstract type: Field:R3 → Real

---

R3 → Real Field constant in space.

`TYPE` = <*selection: Field:R3 → Real_TYPE_selection*>

Default: FieldElementwise []

Sub-record selection.

`gmsh_file` = <*input file name*>

Default: <*obligatory*> []

Input file with ASCII GMSH file format.

`field_name` = *<String (generic)>*

Default: *<obligatory>* []

The values of the Field are read from the $ElementData section with field name given by this key.

---

record: **FieldInterpolatedP0** implements abstract type: Field:R3 → Real

---

Field given by P0 data on another mesh. Currently defined only on boundary.

`TYPE` = *<selection: Field:R3 → Real_TYPE_selection>*

Default: FieldInterpolatedP0 []

Sub-record selection.

`mesh` = *<input file name>*

Default: *<obligatory>* []

File with the mesh from which we interpolate. (currently only GMSH supported)

`raw_data` = *<input file name>*

Default: *<obligatory>* []

File with raw output from flow calculation. Currently we can interpolate only pressure.

---

abstract type: **Field:R3 → Real** default descendant: FieldConstant

---

Descendants:

Abstract record for all time-space functions.

`FieldConstant`

`FieldFormula`

`FieldPython`

`FieldElementwise`

---

record: **FieldConstant** implements abstract type: Field:R3 → Real constructible from key: value

---

R3 → Real Field constant in space.

`TYPE` = *<selection: Field:R3 → Real_TYPE_selection>*

Default: FieldConstant []

Sub-record selection.

`value` = *<Double >*

Default: *<obligatory>* []

Value of the constant field. For vector values, you can use scalar value to enter

constant vector. For square NxN-matrix values, you can use: * vector of size N to enter diagonal matrix * vector of size (N+1)*N/2 to enter symmetric matrix (upper triangle, row by row) * scalar to enter multiple of the unit matrix.

---

record: **FieldFormula** implements abstract type: Field:R3 → Real

---

R3 → Real Field given by runtime interpreted formula.

`TYPE` = <*selection: Field:R3 → Real_TYPE_selection*>

Default: FieldFormula []

Sub-record selection.

`value` = <*String (generic)*>

Default: <*obligatory*> []

String, array of strings, or matrix of strings with formulas for individual entries of scalar, vector, or tensor value respectively. For vector values, you can use just one string to enter homogeneous vector. For square NxN-matrix values, you can use: * array of strings of size N to enter diagonal matrix * array of strings of size (N+1)*N/2 to enter symmetric matrix (upper triangle, row by row) * just one string to enter (spatially variable) multiple of the unit matrix. Formula can contain variables x,y,z,t and usual operators and functions.

---

record: **FieldPython** implements abstract type: Field:R3 → Real

---

R3 → Real Field given by a Python script.

`TYPE` = <*selection: Field:R3 → Real_TYPE_selection*>

Default: FieldPython []

Sub-record selection.

`script_string` = <*String (generic)*>

Default: "Obligatory if 'script_file' is not given." []

Python script given as in place string

`script_file` = <*input file name*>

Default: "Obligatory if 'script_striong' is not given." []

Python script given as external file

`function` = <*String (generic)*>

Default: <*obligatory*> []

Function in the given script that returns tuple containing components of the return type. For NxM tensor values: tensor(row,col) = tuple(M*row + col).

---

record: **FieldElementwise** implements abstract type: Field:R3 → Real

---

R3 → Real Field constant in space.

`TYPE` = <*selection: Field:R3 → Real_TYPE_selection*>

Default: FieldElementwise []

Sub-record selection.

`gmsh_file` = <*input file name*>

Default: <*obligatory*> []

Input file with ASCII GMSH file format.

`field_name` = <*String (generic)*>

Default: <*obligatory*> []

The values of the Field are read from the $ElementData section with field name given by this key.

---

record: **DarcyFlowMH_Steady_BulkData**

Record to set BULK fields of the equation 'DarcyFlowMH_Steady'. The fields are set only on the domain specified by one of the keys: 'region', 'rid', 'r_set' and after the time given by the key 'time'. The field setting can be overridden by any DarcyFlowMH_Steady_BulkData record that comes later in the bulk data array.

`r_set` = <*String (generic)*>

Default: <*optional*> []

Name of region set where to set fields.

`region` = <*String (generic)*>

Default: <*optional*> []

Label of the region where to set fields.

`rid` = <*Integer [0,]*>

Default: <*optional*> []

ID of the region where to set fields.

`time` = <*Double [0,]*>

Default: 0.0 []

Apply field setting in this record after this time. These times has to form an increasing sequence.

`anisotropy` = <*abstract type: Field:R3 → Real[3,3]*>

Default: <*optional*> []

Anisothropic conductivity tensor.

`cross_section` = <*abstract type: Field:R3 → Real*>

Default: <*optional*> []

Complement dimension parameter (cross section for 1D, thickness for 2D).

`conductivity` = <*abstract type: Field:R3 → Real*>

Default: <*optional*> []

Isothropic conductivity scalar.

`sigma` = <*abstract type: Field:R3 → Real*>

Default: <*optional*> []

Transition coefficient between dimensions.

`water_source_density` = <*abstract type: Field:R3 → Real*>

Default: <*optional*> []

Water source density.

`init_pressure` = <*abstract type: Field:R3 → Real*>

Default: <*optional*> []

Initial condition as pressure

`storativity` = <*abstract type: Field:R3 → Real*>

Default: <*optional*> []

Storativity.

`init_piezo_head` = <*abstract type: Field:R3 → Real*>

Default: <*optional*> []

Initial condition for pressure as piezometric head.

---

abstract type: **Field:R3 → Real[3,3]** default descendant: FieldConstant

---

Descendants:

Abstract record for all time-space functions.

`FieldConstant`

`FieldPython`

`FieldFormula`

`FieldElementwise`

`FieldInterpolatedP0`

---

record: **FieldConstant** implements abstract type: Field:R3 → Real[3,3] constructible from key: value

---

R3 → Real[3,3] Field constant in space.

`TYPE` = <*selection: Field:R3 → Real[3,3]_TYPE_selection*>

Default: FieldConstant []

Sub-record selection.

`value` = <*Array [1,] of Array [1,] of Double* >

Default: <*obligatory*> []

Value of the constant field. For vector values, you can use scalar value to enter constant vector. For square NxN-matrix values, you can use: * vector of size N to enter diagonal matrix * vector of size (N+1)*N/2 to enter symmetric matrix (upper triangle, row by row) * scalar to enter multiple of the unit matrix.

---

record: **FieldPython** implements abstract type: Field:R3 → Real[3,3]

R3 → Real[3,3] Field given by a Python script.

`TYPE` = *<selection: Field:R3 → Real[3,3]_TYPE_selection>*

Default: FieldPython []

Sub-record selection.

`script_string` = *<String (generic)>*

Default: "Obligatory if 'script_file' is not given." []

Python script given as in place string

`script_file` = *<input file name>*

Default: "Obligatory if 'script_striong' is not given." []

Python script given as external file

`function` = *<String (generic)>*

Default: *<obligatory>* []

Function in the given script that returns tuple containing components of the return type. For NxM tensor values: tensor(row,col) = tuple(M*row + col).

---

record: **FieldFormula** implements abstract type: Field:R3 → Real[3,3]

R3 → Real[3,3] Field given by runtime interpreted formula.

`TYPE` = *<selection: Field:R3 → Real[3,3]_TYPE_selection>*

Default: FieldFormula []

Sub-record selection.

`value` = *<Array [1,] of Array [1,] of String (generic)>*

Default: *<obligatory>* []

String, array of strings, or matrix of strings with formulas for individual entries of scalar, vector, or tensor value respectively. For vector values, you can use just one string to enter homogeneous vector. For square NxN-matrix values, you can use: * array of strings of size N to enter diagonal matrix * array of strings of size (N+1)*N/2 to enter symmetric matrix (upper triangle, row by row) * just one string to enter (spatially variable) multiple of the unit matrix. Formula can contain variables x,y,z,t and usual operators and functions.

---

record: **FieldElementwise** implements abstract type: Field:R3 → Real[3,3]

R3 → Real[3,3] Field constant in space.

`TYPE` = *<selection: Field:R3 → Real[3,3]_TYPE_selection>*

Default: FieldElementwise []

Sub-record selection.

`gmsh_file` = *<input file name>*

Default: *<obligatory>* []

Input file with ASCII GMSH file format.

`field_name` = *<String (generic)>*

Default: *<obligatory>* []

The values of the Field are read from the $ElementData section with field name given by this key.

---

record: **FieldInterpolatedP0** implements abstract type: Field:R3 → Real[3,3]

Field given by P0 data on another mesh. Currently defined only on boundary.

`TYPE` = *<selection: Field:R3 → Real[3,3]_TYPE_selection>*

Default: FieldInterpolatedP0 []

Sub-record selection.

`mesh` = *<input file name>*

Default: *<obligatory>* []

File with the mesh from which we interpolate. (currently only GMSH supported)

`raw_data` = *<input file name>*

Default: *<obligatory>* []

File with raw output from flow calculation. Currently we can interpolate only pressure.

---

abstract type: **Field:R3 → Real** default descendant: FieldConstant

---

Descendants:

Abstract record for all time-space functions.

`FieldConstant`

`FieldFormula`

`FieldPython`

`FieldElementwise`

---

record: **FieldConstant** implements abstract type: Field:R3 → Real constructible from key: value

---

R3 → Real Field constant in space.

`TYPE` = *<selection: Field:R3 → Real_TYPE_selection>*

Default: FieldConstant []

Sub-record selection.

`value` = *<Double >*

Default: *<obligatory>* []

Value of the constant field. For vector values, you can use scalar value to enter constant vector. For square NxN-matrix values, you can use: * vector of size N to enter diagonal matrix * vector of size (N+1)*N/2 to enter symmetric matrix (upper triangle, row by row) * scalar to enter multiple of the unit matrix.

---

record: **FieldFormula** implements abstract type: Field:R3 → Real

---

R3 → Real Field given by runtime interpreted formula.

`TYPE` = *<selection: Field:R3 → Real_TYPE_selection>*

Default: FieldFormula []

Sub-record selection.

`value` = *<String (generic)>*

Default: *<obligatory>* []

String, array of strings, or matrix of strings with formulas for individual entries of scalar, vector, or tensor value respectively. For vector values, you can use just one string to enter homogeneous vector. For square NxN-matrix values, you can use: * array of strings of size N to enter diagonal matrix * array of strings of size (N+1)*N/2 to enter symmetric matrix (upper triangle, row by row) * just one string to enter (spatially variable) multiple of the unit matrix. Formula can contain variables x,y,z,t and usual operators and functions.

---

record: **FieldPython** implements abstract type: Field:R3 → Real

---

R3 → Real Field given by a Python script.

`TYPE` = *<selection: Field:R3 → Real_TYPE_selection>*

Default: FieldPython []

Sub-record selection.

`script_string` = *<String (generic)>*

Default: "Obligatory if 'script_file' is not given." []

Python script given as in place string

`script_file` = *<input file name>*

Default: "Obligatory if 'script_striong' is not given." []

Python script given as external file

`function` = *<String (generic)>*

Default: <*obligatory*> []

Function in the given script that returns tuple containing components of the return type. For NxM tensor values: tensor(row,col) = tuple(M*row + col).

---

record: **FieldElementwise** implements abstract type: Field:R3 → Real

---

R3 → Real Field constant in space.

`TYPE` = <*selection: Field:R3 → Real_TYPE_selection*>

Default: FieldElementwise []

Sub-record selection.

`gmsh_file` = <*input file name*>

Default: <*obligatory*> []

Input file with ASCII GMSH file format.

`field_name` = <*String (generic)*>

Default: <*obligatory*> []

The values of the Field are read from the $ElementData section with field name given by this key.

---

record: **Unsteady_MH** implements abstract type: DarcyFlowMH

Mixed-Hybrid solver for unsteady saturated Darcy flow.

`TYPE` = <*selection: DarcyFlowMH_TYPE_selection*>

Default: Unsteady_MH []

Sub-record selection.

`n_schurs` = <*Integer [0, 2]*>

Default: 2 []

Number of Schur complements to perform when solving MH sytem.

`solver` = <*abstract type: Solver*>

Default: <*obligatory*> []

Linear solver for MH problem.

`output` = <*record: DarcyMHOutput*>

Default: <*obligatory*> []

Parameters of output form MH module.

`mortar_method` = <*selection: MH_MortarMethod*>

Default: None []

Method for coupling Darcy flow between dimensions.

`mortar_sigma` = <*Double [0,]*>

Default: 1.0 []

Conductivity between dimensions.

`time` = <*record: TimeGovernor*>

Default: <*obligatory*> []

Time governor setting for the unsteady Darcy flow model.

`bc_data` = <*Array of record: DarcyFlowMH_Steady_BoundaryData*>

Default: <*obligatory*> []

`bulk_data` = <*Array of record: DarcyFlowMH_Steady_BulkData*>

Default: <*obligatory*> []

---

record: **DarcyFlowMH_Steady_BoundaryData**

Record to set BOUNDARY fields of the equation 'DarcyFlowMH_Steady'. The fields are set only on the domain specified by one of the keys: 'region', 'rid', 'r_set' and after the time given by the key 'time'. The field setting can be overridden by any DarcyFlowMH_Steady_BoundaryData record that comes later in the boundary data array.

`r_set` = <*String (generic)*>

Default: <*optional*> []

Name of region set where to set fields.

`region` = <*String (generic)*>

Default: <*optional*> []

Label of the region where to set fields.

`rid` = <*Integer [0,]*>

Default: <*optional*> []

ID of the region where to set fields.

`time` = <*Double [0,]*>

Default: 0.0 []

Apply field setting in this record after this time. These times has to form an increasing sequence.

`bc_type` = <*abstract type: Field:R3 → Enum*>

Default: <*optional*> []

Boundary condition type, possible values:

`bc_pressure` = <*abstract type: Field:R3 → Real*>

Default: <*optional*> []

Dirichlet BC condition value for pressure.

`bc_flux` = <*abstract type: Field:R3 → Real*>

Default: <*optional*> []

Flux in Neumman or Robin boundary condition.

`bc_robin_sigma` = <*abstract type: Field:R3 → Real*>

Default: <*optional*> []

Conductivity coefficient in Robin boundary condition.

`bc_piezo_head` = <*abstract type: Field:R3 → Real*>

Default: <*optional*> []

Boundary condition for piezometric head.

`flow_old_bcd_file` = <*input file name*>

Default: <*optional*> []

---

abstract type: **Field:R3 → Enum** default descendant: FieldConstant

---

Descendants:

Abstract record for all time-space functions.

`FieldConstant`

`FieldFormula`

`FieldPython`

`FieldElementwise`

---

record: **FieldConstant** implements abstract type: Field:R3 → Enum constructible from key: value

---

R3 → Enum Field constant in space.

`TYPE` = <*selection: Field:R3 → Enum_TYPE_selection*>

Default: FieldConstant []

Sub-record selection.

`value` = <*selection: EqData_bc_Type*>

Default: <*obligatory*> []

Value of the constant field. For vector values, you can use scalar value to enter constant vector. For square NxN-matrix values, you can use: * vector of size N to enter diagonal matrix * vector of size (N+1)*N/2 to enter symmetric matrix (upper triangle, row by row) * scalar to enter multiple of the unit matrix.

---

record: **FieldFormula** implements abstract type: Field:R3 → Enum

---

R3 → Enum Field given by runtime interpreted formula.

`TYPE` = <*selection: Field:R3 → Enum_TYPE_selection*>

Default: FieldFormula []

Sub-record selection.

`value` = *<String (generic)>*

Default: *<obligatory>* []

String, array of strings, or matrix of strings with formulas for individual entries of scalar, vector, or tensor value respectively. For vector values, you can use just one string to enter homogeneous vector. For square NxN-matrix values, you can use: * array of strings of size N to enter diagonal matrix * array of strings of size (N+1)*N/2 to enter symmetric matrix (upper triangle, row by row) * just one string to enter (spatially variable) multiple of the unit matrix. Formula can contain variables x,y,z,t and usual operators and functions.

---

record: **FieldPython** implements abstract type: Field:R3 → Enum

---

R3 → Enum Field given by a Python script.

`TYPE` = *<selection: Field:R3 → Enum_TYPE_selection>*

Default: FieldPython []

Sub-record selection.

`script_string` = *<String (generic)>*

Default: "Obligatory if 'script_file' is not given." []

Python script given as in place string

`script_file` = *<input file name>*

Default: "Obligatory if 'script_striong' is not given." []

Python script given as external file

`function` = *<String (generic)>*

Default: *<obligatory>* []

Function in the given script that returns tuple containing components of the return type. For NxM tensor values: tensor(row,col) = tuple(M*row + col).

---

record: **FieldElementwise** implements abstract type: Field:R3 → Enum

---

R3 → Enum Field constant in space.

`TYPE` = *<selection: Field:R3 → Enum_TYPE_selection>*

Default: FieldElementwise []

Sub-record selection.

`gmsh_file` = *<input file name>*

Default: *<obligatory>* []

Input file with ASCII GMSH file format.

`field_name` = *<String (generic)>*

Default: *<obligatory>* []

The values of the Field are read from the $ElementData section with field name given by this key.

---

abstract type: **Field:R3 → Real** default descendant: FieldConstant

---

Descendants:

Abstract record for all time-space functions.

FieldConstant

FieldFormula

FieldPython

FieldElementwise

---

record: **FieldConstant** implements abstract type: Field:R3 → Real constructible from key: value

---

R3 → Real Field constant in space.

`TYPE` = *<selection: Field:R3 → Real_TYPE_selection>*

Default: FieldConstant []

Sub-record selection.

`value` = *<Double >*

Default: *<obligatory>* []

Value of the constant field. For vector values, you can use scalar value to enter constant vector. For square NxN-matrix values, you can use: * vector of size N to enter diagonal matrix * vector of size (N+1)*N/2 to enter symmetric matrix (upper triangle, row by row) * scalar to enter multiple of the unit matrix.

---

record: **FieldFormula** implements abstract type: Field:R3 → Real

---

R3 → Real Field given by runtime interpreted formula.

`TYPE` = *<selection: Field:R3 → Real_TYPE_selection>*

Default: FieldFormula []

Sub-record selection.

`value` = *<String (generic)>*

Default: *<obligatory>* []

String, array of strings, or matrix of strings with formulas for individual entries of scalar, vector, or tensor value respectively. For vector values, you can use just one string to enter homogeneous vector. For square NxN-matrix values, you can use: * array of strings of size N to enter diagonal matrix * array of strings of size (N+1)*N/2 to enter symmetric matrix (upper triangle, row by row) * just one string to enter (spatially variable) multiple of the unit matrix. Formula can contain variables x,y,z,t and usual operators and functions.

record: **FieldPython** implements abstract type: Field:R3 → Real

R3 → Real Field given by a Python script.

`TYPE` = *<selection: Field:R3 → Real_TYPE_selection>*

Default: FieldPython []

Sub-record selection.

`script_string` = *<String (generic)>*

Default: "Obligatory if 'script_file' is not given." []

Python script given as in place string

`script_file` = *<input file name>*

Default: "Obligatory if 'script_striong' is not given." []

Python script given as external file

`function` = *<String (generic)>*

Default: *<obligatory>* []

Function in the given script that returns tuple containing components of the return type. For NxM tensor values: tensor(row,col) = tuple(M*row + col).

record: **FieldElementwise** implements abstract type: Field:R3 → Real

R3 → Real Field constant in space.

`TYPE` = *<selection: Field:R3 → Real_TYPE_selection>*

Default: FieldElementwise []

Sub-record selection.

`gmsh_file` = *<input file name>*

Default: *<obligatory>* []

Input file with ASCII GMSH file format.

`field_name` = *<String (generic)>*

Default: *<obligatory>* []

The values of the Field are read from the $ElementData section with field name given by this key.

record: **DarcyFlowMH_Steady_BulkData**

Record to set BULK fields of the equation 'DarcyFlowMH_Steady'. The fields are set only on the domain specified by one of the keys: 'region', 'rid', 'r_set' and after the time given by the key 'time'. The field setting can be overridden by any DarcyFlowMH_Steady_BulkData record that comes later in the bulk data array.

`r_set` = *<String (generic)>*

Default: <*optional*> []

Name of region set where to set fields.

`region` = <*String (generic)*>

Default: <*optional*> []

Label of the region where to set fields.

`rid` = <*Integer [0,]*>

Default: <*optional*> []

ID of the region where to set fields.

`time` = <*Double [0,]*>

Default: 0.0 []

Apply field setting in this record after this time. These times has to form an increasing sequence.

`anisotropy` = <*abstract type: Field:R3 → Real[3,3]*>

Default: <*optional*> []

Anisothropic conductivity tensor.

`cross_section` = <*abstract type: Field:R3 → Real*>

Default: <*optional*> []

Complement dimension parameter (cross section for 1D, thickness for 2D).

`conductivity` = <*abstract type: Field:R3 → Real*>

Default: <*optional*> []

Isothropic conductivity scalar.

`sigma` = <*abstract type: Field:R3 → Real*>

Default: <*optional*> []

Transition coefficient between dimensions.

`water_source_density` = <*abstract type: Field:R3 → Real*>

Default: <*optional*> []

Water source density.

`init_pressure` = <*abstract type: Field:R3 → Real*>

Default: <*optional*> []

Initial condition as pressure

`storativity` = <*abstract type: Field:R3 → Real*>

Default: <*optional*> []

Storativity.

`init_piezo_head` = <*abstract type: Field:R3 → Real*>

Default: <*optional*> []

Initial piezometric head.

---

abstract type: **Field:R3 → Real** default descendant: FieldConstant

---

Descendants:

Abstract record for all time-space functions.

FieldConstant

FieldFormula

FieldPython

FieldElementwise

---

record: **FieldConstant** implements abstract type: Field:R3 → Real constructible from key: value

---

R3 → Real Field constant in space.

`TYPE` = *<selection: Field:R3 → Real_TYPE_selection>*

Default: FieldConstant []

Sub-record selection.

`value` = *<Double >*

Default: *<obligatory>* []

Value of the constant field. For vector values, you can use scalar value to enter constant vector. For square NxN-matrix values, you can use: * vector of size N to enter diagonal matrix * vector of size (N+1)*N/2 to enter symmetric matrix (upper triangle, row by row) * scalar to enter multiple of the unit matrix.

---

record: **FieldFormula** implements abstract type: Field:R3 → Real

---

R3 → Real Field given by runtime interpreted formula.

`TYPE` = *<selection: Field:R3 → Real_TYPE_selection>*

Default: FieldFormula []

Sub-record selection.

`value` = *<String (generic)>*

Default: *<obligatory>* []

String, array of strings, or matrix of strings with formulas for individual entries of scalar, vector, or tensor value respectively. For vector values, you can use just one string to enter homogeneous vector. For square NxN-matrix values, you can use: * array of strings of size N to enter diagonal matrix * array of strings of size (N+1)*N/2 to enter symmetric matrix (upper triangle, row by row) * just one string to enter (spatially variable) multiple of the unit matrix. Formula can contain variables x,y,z,t and usual operators and functions.

---

record: **FieldPython** implements abstract type: Field:R3 → Real

R3 → Real Field given by a Python script.

`TYPE` = *<selection: Field:R3 → Real_TYPE_selection>*

Default: FieldPython []

Sub-record selection.

`script_string` = *<String (generic)>*

Default: "Obligatory if 'script_file' is not given." []

Python script given as in place string

`script_file` = *<input file name>*

Default: "Obligatory if 'script_striong' is not given." []

Python script given as external file

`function` = *<String (generic)>*

Default: *<obligatory>* []

Function in the given script that returns tuple containing components of the return type. For NxM tensor values: tensor(row,col) = tuple(M*row + col).

---

record: **FieldElementwise** implements abstract type: Field:R3 → Real

R3 → Real Field constant in space.

`TYPE` = *<selection: Field:R3 → Real_TYPE_selection>*

Default: FieldElementwise []

Sub-record selection.

`gmsh_file` = *<input file name>*

Default: *<obligatory>* []

Input file with ASCII GMSH file format.

`field_name` = *<String (generic)>*

Default: *<obligatory>* []

The values of the Field are read from the $ElementData section with field name given by this key.

---

record: **Unsteady_LMH** implements abstract type: DarcyFlowMH

Lumped Mixed-Hybrid solver for unsteady saturated Darcy flow.

`TYPE` = *<selection: DarcyFlowMH_TYPE_selection>*

Default: Unsteady_LMH []

Sub-record selection.

`n_schurs` = *<Integer [0, 2]>*

Default: 2 []

Number of Schur complements to perform when solving MH sytem.

`solver` = <*abstract type: Solver*>

Default: <*obligatory*> []

Linear solver for MH problem.

`output` = <*record: DarcyMHOutput*>

Default: <*obligatory*> []

Parameters of output form MH module.

`mortar_method` = <*selection: MH_MortarMethod*>

Default: None []

Method for coupling Darcy flow between dimensions.

`mortar_sigma` = <*Double [0,]*>

Default: 1.0 []

Conductivity between dimensions.

`time` = <*record: TimeGovernor*>

Default: <*obligatory*> []

Time governor setting for the unsteady Darcy flow model.

`bc_data` = <*Array of record: DarcyFlowMH_Steady_BoundaryData*>

Default: <*obligatory*> []

`bulk_data` = <*Array of record: DarcyFlowMH_Steady_BulkData*>

Default: <*obligatory*> []

---

record: **DarcyFlowMH_Steady_BoundaryData**

Record to set BOUNDARY fields of the equation 'DarcyFlowMH_Steady'. The fields are set only on the domain specified by one of the keys: 'region', 'rid', 'r_set' and after the time given by the key 'time'. The field setting can be overridden by any DarcyFlowMH_Steady_BoundaryData record that comes later in the boundary data array.

`r_set` = <*String (generic)*>

Default: <*optional*> []

Name of region set where to set fields.

`region` = <*String (generic)*>

Default: <*optional*> []

Label of the region where to set fields.

`rid` = <*Integer [0,]*>

Default: <*optional*> []

ID of the region where to set fields.

`time` = <*Double [0,]*>

Default: 0.0 []

Apply field setting in this record after this time. These times has to form an increasing sequence.

`bc_type` = <*abstract type: Field:R3 → Enum*>

Default: <*optional*> []

Boundary condition type, possible values:

`bc_pressure` = <*abstract type: Field:R3 → Real*>

Default: <*optional*> []

Dirichlet BC condition value for pressure.

`bc_flux` = <*abstract type: Field:R3 → Real*>

Default: <*optional*> []

Flux in Neumman or Robin boundary condition.

`bc_robin_sigma` = <*abstract type: Field:R3 → Real*>

Default: <*optional*> []

Conductivity coefficient in Robin boundary condition.

`bc_piezo_head` = <*abstract type: Field:R3 → Real*>

Default: <*optional*> []

Boundary condition for piezometric head.

`flow_old_bcd_file` = <*input file name*>

Default: <*optional*> []

---

abstract type: **Field:R3 → Enum** default descendant: FieldConstant

---

Descendants:

Abstract record for all time-space functions.

`FieldConstant`

`FieldFormula`

`FieldPython`

`FieldElementwise`

---

record: **FieldConstant** implements abstract type: Field:R3 → Enum constructible from key: value

---

R3 → Enum Field constant in space.

`TYPE` = <*selection: Field:R3 → Enum_TYPE_selection*>

Default: FieldConstant []

Sub-record selection.

`value` = <*selection: EqData_bc_Type*>

Default: <*obligatory*> []

Value of the constant field. For vector values, you can use scalar value to enter constant vector. For square NxN-matrix values, you can use: * vector of size N to enter diagonal matrix * vector of size (N+1)*N/2 to enter symmetric matrix (upper triangle, row by row) * scalar to enter multiple of the unit matrix.

---

record: **FieldFormula** implements abstract type: Field:R3 → Enum

---

R3 → Enum Field given by runtime interpreted formula.

`TYPE` = <*selection: Field:R3 → Enum_TYPE_selection*>

Default: FieldFormula []

Sub-record selection.

`value` = <*String (generic)*>

Default: <*obligatory*> []

String, array of strings, or matrix of strings with formulas for individual entries of scalar, vector, or tensor value respectively. For vector values, you can use just one string to enter homogeneous vector. For square NxN-matrix values, you can use: * array of strings of size N to enter diagonal matrix * array of strings of size (N+1)*N/2 to enter symmetric matrix (upper triangle, row by row) * just one string to enter (spatially variable) multiple of the unit matrix. Formula can contain variables x,y,z,t and usual operators and functions.

---

record: **FieldPython** implements abstract type: Field:R3 → Enum

---

R3 → Enum Field given by a Python script.

`TYPE` = <*selection: Field:R3 → Enum_TYPE_selection*>

Default: FieldPython []

Sub-record selection.

`script_string` = <*String (generic)*>

Default: "Obligatory if 'script_file' is not given." []

Python script given as in place string

`script_file` = <*input file name*>

Default: "Obligatory if 'script_striong' is not given." []

Python script given as external file

`function` = <*String (generic)*>

Default: <*obligatory*> []

Function in the given script that returns tuple containing components of the return type. For NxM tensor values: tensor(row,col) = tuple(M*row + col).

record: **FieldElementwise** implements abstract type: Field:R3 → Enum

R3 → Enum Field constant in space.

`TYPE` = <*selection: Field:R3 → Enum_TYPE_selection*>

Default: FieldElementwise []

Sub-record selection.

`gmsh_file` = <*input file name*>

Default: <*obligatory*> []

Input file with ASCII GMSH file format.

`field_name` = <*String (generic)*>

Default: <*obligatory*> []

The values of the Field are read from the $ElementData section with field name given by this key.

---

abstract type: **Field:R3 → Real** default descendant: FieldConstant

Descendants:

Abstract record for all time-space functions.

`FieldConstant`

`FieldFormula`

`FieldPython`

`FieldElementwise`

---

record: **FieldConstant** implements abstract type: Field:R3 → Real constructible from key: value

R3 → Real Field constant in space.

`TYPE` = <*selection: Field:R3 → Real_TYPE_selection*>

Default: FieldConstant []

Sub-record selection.

`value` = <*Double* >

Default: <*obligatory*> []

Value of the constant field. For vector values, you can use scalar value to enter constant vector. For square NxN-matrix values, you can use: * vector of size N to enter diagonal matrix * vector of size (N+1)*N/2 to enter symmetric matrix (upper triangle, row by row) * scalar to enter multiple of the unit matrix.

---

record: **FieldFormula** implements abstract type: Field:R3 → Real

R3 → Real Field given by runtime interpreted formula.

`TYPE` = *<selection: Field:R3 → Real_TYPE_selection>*

Default: FieldFormula []

Sub-record selection.

`value` = *<String (generic)>*

Default: *<obligatory>* []

String, array of strings, or matrix of strings with formulas for individual entries of scalar, vector, or tensor value respectively. For vector values, you can use just one string to enter homogeneous vector. For square NxN-matrix values, you can use: * array of strings of size N to enter diagonal matrix * array of strings of size (N+1)*N/2 to enter symmetric matrix (upper triangle, row by row) * just one string to enter (spatially variable) multiple of the unit matrix. Formula can contain variables x,y,z,t and usual operators and functions.

---

record: **FieldPython** implements abstract type: Field:R3 → Real

---

R3 → Real Field given by a Python script.

`TYPE` = *<selection: Field:R3 → Real_TYPE_selection>*

Default: FieldPython []

Sub-record selection.

`script_string` = *<String (generic)>*

Default: "Obligatory if 'script_file' is not given." []

Python script given as in place string

`script_file` = *<input file name>*

Default: "Obligatory if 'script_striong' is not given." []

Python script given as external file

`function` = *<String (generic)>*

Default: *<obligatory>* []

Function in the given script that returns tuple containing components of the return type. For NxM tensor values: tensor(row,col) = tuple(M*row + col).

---

record: **FieldElementwise** implements abstract type: Field:R3 → Real

---

R3 → Real Field constant in space.

`TYPE` = *<selection: Field:R3 → Real_TYPE_selection>*

Default: FieldElementwise []

Sub-record selection.

`gmsh_file` = *<input file name>*

Default: *<obligatory>* []

Input file with ASCII GMSH file format.

`field_name` = *<String (generic)>*

Default: *<obligatory>* []

The values of the Field are read from the $ElementData section with field name given by this key.

---

record: **DarcyFlowMH_Steady_BulkData**

Record to set BULK fields of the equation 'DarcyFlowMH_Steady'. The fields are set only on the domain specified by one of the keys: 'region', 'rid', 'r_set' and after the time given by the key 'time'. The field setting can be overridden by any DarcyFlowMH_Steady_BulkData record that comes later in the bulk data array.

`r_set` = *<String (generic)>*

Default: *<optional>* []

Name of region set where to set fields.

`region` = *<String (generic)>*

Default: *<optional>* []

Label of the region where to set fields.

`rid` = *<Integer [0,]>*

Default: *<optional>* []

ID of the region where to set fields.

`time` = *<Double [0,]>*

Default: 0.0 []

Apply field setting in this record after this time. These times has to form an increasing sequence.

`anisotropy` = *<abstract type: Field:R3 → Real[3,3]>*

Default: *<optional>* []

Anisothropic conductivity tensor.

`cross_section` = *<abstract type: Field:R3 → Real>*

Default: *<optional>* []

Complement dimension parameter (cross section for 1D, thickness for 2D).

`conductivity` = *<abstract type: Field:R3 → Real>*

Default: *<optional>* []

Isothropic conductivity scalar.

`sigma` = *<abstract type: Field:R3 → Real>*

Default: *<optional>* []

Transition coefficient between dimensions.

`water_source_density` = *<abstract type: Field:R3 → Real>*

Default: <*optional*> []

Water source density.

`init_pressure` = <*abstract type: Field:R3 → Real*>

Default: <*optional*> []

Initial condition as pressure

`storativity` = <*abstract type: Field:R3 → Real*>

Default: <*optional*> []

Storativity.

`init_piezo_head` = <*abstract type: Field:R3 → Real*>

Default: <*optional*> []

Initial piezometric head.

---

abstract type: **Field:R3 → Real** default descendant: FieldConstant

---

Descendants:

Abstract record for all time-space functions.

`FieldConstant`

`FieldFormula`

`FieldPython`

`FieldElementwise`

---

record: **FieldConstant** implements abstract type: Field:R3 → Real constructible from key: value

---

R3 → Real Field constant in space.

`TYPE` = <*selection: Field:R3 → Real_TYPE_selection*>

Default: FieldConstant []

Sub-record selection.

`value` = <*Double* >

Default: <*obligatory*> []

Value of the constant field. For vector values, you can use scalar value to enter constant vector. For square NxN-matrix values, you can use: * vector of size N to enter diagonal matrix * vector of size (N+1)*N/2 to enter symmetric matrix (upper triangle, row by row) * scalar to enter multiple of the unit matrix.

---

record: **FieldFormula** implements abstract type: Field:R3 → Real

---

R3 → Real Field given by runtime interpreted formula.

`TYPE` = <*selection: Field:R3 → Real_TYPE_selection*>

Default: FieldFormula []

Sub-record selection.

`value` = *<String (generic)>*

Default: *<obligatory>* []

String, array of strings, or matrix of strings with formulas for individual entries of scalar, vector, or tensor value respectively. For vector values, you can use just one string to enter homogeneous vector. For square NxN-matrix values, you can use: * array of strings of size N to enter diagonal matrix * array of strings of size (N+1)*N/2 to enter symmetric matrix (upper triangle, row by row) * just one string to enter (spatially variable) multiple of the unit matrix. Formula can contain variables x,y,z,t and usual operators and functions.

---

record: **FieldPython** implements abstract type: Field:R3 → Real

---

R3 → Real Field given by a Python script.

`TYPE` = *<selection: Field:R3 → Real_TYPE_selection>*

Default: FieldPython []

Sub-record selection.

`script_string` = *<String (generic)>*

Default: "Obligatory if 'script_file' is not given." []

Python script given as in place string

`script_file` = *<input file name>*

Default: "Obligatory if 'script_striong' is not given." []

Python script given as external file

`function` = *<String (generic)>*

Default: *<obligatory>* []

Function in the given script that returns tuple containing components of the return type. For NxM tensor values: tensor(row,col) = tuple(M*row + col).

---

record: **FieldElementwise** implements abstract type: Field:R3 → Real

---

R3 → Real Field constant in space.

`TYPE` = *<selection: Field:R3 → Real_TYPE_selection>*

Default: FieldElementwise []

Sub-record selection.

`gmsh_file` = *<input file name>*

Default: *<obligatory>* []

Input file with ASCII GMSH file format.

`field_name` = *<String (generic)>*

Default: <*obligatory*> []

The values of the Field are read from the $ElementData section with field name given by this key.

---

abstract type: **Transport**

Descendants:

Secondary equation for transport of substances.

TransportOperatorSplitting

AdvectionDiffusion_DG

---

record: **TransportOperatorSplitting** implements abstract type: Transport

---

Explicit FVM transport (no diffusion) coupled with reaction and sorption model (ODE per element) via. operator splitting.

`TYPE` = <*selection: Transport_TYPE_selection*>

Default: TransportOperatorSplitting []

Sub-record selection.

`time` = <*record: TimeGovernor*>

Default: <*obligatory*> []

Time governor setting for the transport model.

`substances` = <*Array of String (generic)*>

Default: <*obligatory*> []

Names of transported substances.

`sorption_enable` = <*Bool*>

Default: false []

Model of sorption.

`dual_porosity` = <*Bool*>

Default: false []

Dual porosity model.

`sources_file` = <*input file name*>

Default: <*optional*> []

File with data for the source term in the transport equation.

`output` = <*record: TransportOutput*>

Default: <*obligatory*> []

Parameters of output stream.

`reactions` = <*abstract type: Reactions*>

Default: <*optional*> []

Initialization of per element reactions.

`bc_data` = <*Array of record: TransportOperatorSplitting_BoundaryData*>

Default: <*obligatory*> []

`bulk_data` = <*Array of record: TransportOperatorSplitting_BulkData*>

Default: <*obligatory*> []

---

record: **TransportOutput**

Output setting for transport equations.

`output_stream` = <*record: OutputStrem*>

Default: <*obligatory*> []

Parameters of output stream.

`save_step` = <*Double [0,]*>

Default: <*obligatory*> []

Interval between outputs.

`output_times` = <*Array of Double [0,]*>

Default: <*optional*> []

Explicit array of output times (can be combined with 'save_step'.

`conc_mobile_p0` = <*String (generic)*>

Default: <*optional*> []

Name of output stream for P0 approximation of the concentration in mobile phase.

`conc_immobile_p0` = <*String (generic)*>

Default: <*optional*> []

Name of output stream for P0 approximation of the concentration in immobile phase.

`conc_mobile_sorbed_p0` = <*String (generic)*>

Default: <*optional*> []

Name of output stream for P0 approximation of the surface concentration of sorbed mobile phase.

`conc_immobile_sorbed_p0` = <*String (generic)*>

Default: <*optional*> []

Name of output stream for P0 approximation of the surface concentration of sorbed immobile phase.

---

abstract type: **Reactions**

Descendants:

Equation for reading information about simple chemical reactions.

LinearReactions

PadeApproximant

Isotope

---

record: **LinearReactions** implements abstract type: Reactions

---

Information for a decision about the way to simulate radioactive decay.

`TYPE` = *<selection: Reactions_TYPE_selection>*

Default: LinearReactions []

Sub-record selection.

`decays` = *<Array of record: Substep>*

Default: *<obligatory>* []

Description of particular decay chain substeps.

`matrix_exp_on` = *<Bool>*

Default: false []

Enables to use Pade approximant of matrix exponential.

---

record: **Substep**

Equation for reading information about radioactive decays.

`parent` = *<String (generic)>*

Default: *<obligatory>* []

Identifier of an isotope.

`half_life` = *<Double >*

Default: *<optional>* []

Half life of the parent substance.

`kinetic` = *<Double >*

Default: *<optional>* []

Kinetic constants describing first order reactions.

`products` = *<Array of String (generic)>*

Default: *<obligatory>* []

Identifies isotopes which decays parental atom to.

`branch_ratios` = *<Array of Double >*

Default: 1.0 []

Decay chain branching percentage.

---

record: **PadeApproximant** implements abstract type: Reactions

Abstract record with an information about pade approximant parameters.

`TYPE` = *<selection: Reactions_TYPE_selection>*

Default: PadeApproximant []

Sub-record selection.

`decays` = *<Array of record: Substep>*

Default: *<obligatory>* []

Description of particular decay chain substeps.

`nom_pol_deg` = *<Integer >*

Default: 2 []

Polynomial degree of the nominator of Pade approximant.

`den_pol_deg` = *<Integer >*

Default: 2 []

Polynomial degree of the nominator of Pade approximant

record: **Substep**

Equation for reading information about radioactive decays.

`parent` = *<String (generic)>*

Default: *<obligatory>* []

Identifier of an isotope.

`half_life` = *<Double >*

Default: *<optional>* []

Half life of the parent substance.

`kinetic` = *<Double >*

Default: *<optional>* []

Kinetic constants describing first order reactions.

`products` = *<Array of String (generic)>*

Default: *<obligatory>* []

Identifies isotopes which decays parental atom to.

`branch_ratios` = *<Array of Double >*

Default: 1.0 []

Decay chain branching percentage.

record: **Isotope** implements abstract type: Reactions

Definition of information about a single isotope.

`TYPE` = <*selection: Reactions_TYPE_selection*>

Default: Isotope []

Sub-record selection.

`identifier` = <*Integer* >

Default: <*obligatory*> []

Identifier of the isotope.

`half_life` = <*Double* >

Default: <*obligatory*> []

Half life parameter.

---

record: **TransportOperatorSplitting_BoundaryData**

Record to set BOUNDARY fields of the equation 'TransportOperatorSplitting'. The fields are set only on the domain specified by one of the keys: 'region', 'rid', 'r_set' and after the time given by the key 'time'. The field setting can be overridden by any TransportOperatorSplitting_BoundaryData record that comes later in the boundary data array.

`r_set` = <*String (generic)*>

Default: <*optional*> []

Name of region set where to set fields.

`region` = <*String (generic)*>

Default: <*optional*> []

Label of the region where to set fields.

`rid` = <*Integer [0,]*>

Default: <*optional*> []

ID of the region where to set fields.

`time` = <*Double [0,]*>

Default: 0.0 []

Apply field setting in this record after this time. These times has to form an increasing sequence.

`bc_conc` = <*abstract type: Field:R3 → Real[n]*>

Default: <*optional*> []

Boundary conditions for concentrations.

`old_boundary_file` = <*input file name*>

Default: <*optional*> []

Input file with boundary conditions (obsolete).

`bc_times` = <*Array of Double* >

Default: <*optional*> []

Times for changing the boundary conditions (obsolete).

---

abstract type: **Field:R3 → Real[n]** default descendant: FieldConstant

---

Descendants:

Abstract record for all time-space functions.

`FieldConstant`

`FieldPython`

`FieldFormula`

`FieldElementwise`

`FieldInterpolatedP0`

---

record: **FieldConstant** implements abstract type: Field:R3 → Real[n] constructible from key: value

---

R3 → Real[n] Field constant in space.

`TYPE` = <*selection: Field:R3 → Real[n]_TYPE_selection*>

Default: FieldConstant []

Sub-record selection.

`value` = <*Array [1,] of Double* >

Default: <*obligatory*> []

Value of the constant field. For vector values, you can use scalar value to enter constant vector. For square NxN-matrix values, you can use: * vector of size N to enter diagonal matrix * vector of size (N+1)*N/2 to enter symmetric matrix (upper triangle, row by row) * scalar to enter multiple of the unit matrix.

---

record: **FieldPython** implements abstract type: Field:R3 → Real[n]

R3 → Real[n] Field given by a Python script.

`TYPE` = <*selection: Field:R3 → Real[n]_TYPE_selection*>

Default: FieldPython []

Sub-record selection.

`script_string` = <*String (generic)*>

Default: "Obligatory if 'script_file' is not given." []

Python script given as in place string

`script_file` = <*input file name*>

Default: "Obligatory if 'script_striong' is not given." []

Python script given as external file

`function` = *<String (generic)>*

Default: *<obligatory>* []

Function in the given script that returns tuple containing components of the return type. For NxM tensor values: tensor(row,col) = tuple(M*row + col).

---

record: **FieldFormula** implements abstract type: Field:R3 → Real[n]

R3 → Real[n] Field given by runtime interpreted formula.

`TYPE` = *<selection: Field:R3 → Real[n]_TYPE_selection>*

Default: FieldFormula []

Sub-record selection.

`value` = *<Array [1,] of String (generic)>*

Default: *<obligatory>* []

String, array of strings, or matrix of strings with formulas for individual entries of scalar, vector, or tensor value respectively. For vector values, you can use just one string to enter homogeneous vector. For square NxN-matrix values, you can use: * array of strings of size N to enter diagonal matrix * array of strings of size (N+1)*N/2 to enter symmetric matrix (upper triangle, row by row) * just one string to enter (spatially variable) multiple of the unit matrix. Formula can contain variables x,y,z,t and usual operators and functions.

---

record: **FieldElementwise** implements abstract type: Field:R3 → Real[n]

R3 → Real[n] Field constant in space.

`TYPE` = *<selection: Field:R3 → Real[n]_TYPE_selection>*

Default: FieldElementwise []

Sub-record selection.

`gmsh_file` = *<input file name>*

Default: *<obligatory>* []

Input file with ASCII GMSH file format.

`field_name` = *<String (generic)>*

Default: *<obligatory>* []

The values of the Field are read from the $ElementData section with field name given by this key.

---

record: **FieldInterpolatedP0** implements abstract type: Field:R3 → Real[n]

Field given by P0 data on another mesh. Currently defined only on boundary.

`TYPE` = *<selection: Field:R3 → Real[n]_TYPE_selection>*

Default: FieldInterpolatedP0 []

Sub-record selection.

`mesh` = *<input file name>*

Default: *<obligatory>* []

File with the mesh from which we interpolate. (currently only GMSH supported)

`raw_data` = *<input file name>*

Default: *<obligatory>* []

File with raw output from flow calculation. Currently we can interpolate only pressure.

---

record: **TransportOperatorSplitting_BulkData**

Record to set BULK fields of the equation 'TransportOperatorSplitting'. The fields are set only on the domain specified by one of the keys: 'region', 'rid', 'r_set' and after the time given by the key 'time'. The field setting can be overridden by any TransportOperatorSplitting_BulkData record that comes later in the bulk data array.

`r_set` = *<String (generic)>*

Default: *<optional>* []

Name of region set where to set fields.

`region` = *<String (generic)>*

Default: *<optional>* []

Label of the region where to set fields.

`rid` = *<Integer [0,]>*

Default: *<optional>* []

ID of the region where to set fields.

`time` = *<Double [0,]>*

Default: 0.0 []

Apply field setting in this record after this time. These times has to form an increasing sequence.

`init_conc` = *<abstract type: Field:R3 → Real[n]>*

Default: *<optional>* []

Initial concentrations.

`por_m` = *<abstract type: Field:R3 → Real>*

Default: *<optional>* []

Mobile porosity

`por_imm` = *<abstract type: Field:R3 → Real>*

Default: *<optional>* []

Immobile porosity

`alpha` = <*abstract type: Field:R3 → Real[n]*>

Default: <*optional*> []

Coefficients of non-equilibrium exchange.

`sorp_type` = <*abstract type: Field:R3 → Real[n]*>

Default: <*optional*> []

Type of sorption.

`sorp_coef0` = <*abstract type: Field:R3 → Real[n]*>

Default: <*optional*> []

Coefficient of sorption.

`sorp_coef1` = <*abstract type: Field:R3 → Real[n]*>

Default: <*optional*> []

Coefficient of sorption.

`phi` = <*abstract type: Field:R3 → Real*>

Default: <*optional*> []

Solid / solid mobile.

`sources_density` = <*abstract type: Field:R3 → Real[n]*>

Default: <*optional*> []

Density of transport sources.

`sources_sigma` = <*abstract type: Field:R3 → Real[n]*>

Default: <*optional*> []

`sources_conc` = <*abstract type: Field:R3 → Real[n]*>

Default: <*optional*> []

Concentration sources.

---

record: **AdvectionDiffusion_DG** implements abstract type: Transport

---

DG solver for transport with diffusion.

`TYPE` = <*selection: Transport_TYPE_selection*>

Default: AdvectionDiffusion_DG []

Sub-record selection.

`time` = <*record: TimeGovernor*>

Default: <*obligatory*> []

Time governor setting for the transport model.

`substances` = <*Array of String (generic)*>

Default: <*obligatory*> []

Names of transported substances.

`sorption_enable` = <*Bool*>

Default: false []

Model of sorption.

`dual_porosity` = <*Bool*>

Default: false []

Dual porosity model.

`sources_file` = <*input file name*>

Default: <*optional*> []

File with data for the source term in the transport equation.

`output` = <*record: TransportOutput*>

Default: <*obligatory*> []

Parameters of output stream.

`solver` = <*abstract type: Solver*>

Default: <*obligatory*> []

Linear solver for MH problem.

`bc_data` = <*Array of record: TransportDG_BoundaryData*>

Default: <*obligatory*> []

`bulk_data` = <*Array of record: TransportDG_BulkData*>

Default: <*obligatory*> []

---

record: **TransportDG_BoundaryData**

Record to set BOUNDARY fields of the equation 'TransportDG'. The fields are set only on the domain specified by one of the keys: 'region', 'rid', 'r_set' and after the time given by the key 'time'. The field setting can be overridden by any TransportDG_BoundaryData record that comes later in the boundary data array.

`r_set` = <*String (generic)*>

Default: <*optional*> []

Name of region set where to set fields.

`region` = <*String (generic)*>

Default: <*optional*> []

Label of the region where to set fields.

`rid` = <*Integer [0,]*>

Default: <*optional*> []

ID of the region where to set fields.

`time` = <*Double [0,]*>

Default: 0.0 []

Apply field setting in this record after this time. These times has to form an increasing sequence.

`bc_conc` = <*abstract type: Field:R3 → Real[n]*>

Default: <*optional*> []

Boundary conditions for concentrations.

`old_boundary_file` = <*input file name*>

Default: <*optional*> []

Input file with boundary conditions (obsolete).

`bc_times` = <*Array of Double* >

Default: <*optional*> []

Times for changing the boundary conditions (obsolete).

---

record: **TransportDG_BulkData**

Record to set BULK fields of the equation 'TransportDG'. The fields are set only on the domain specified by one of the keys: 'region', 'rid', 'r_set' and after the time given by the key 'time'. The field setting can be overridden by any TransportDG_BulkData record that comes later in the bulk data array.

`r_set` = <*String (generic)*>

Default: <*optional*> []

Name of region set where to set fields.

`region` = <*String (generic)*>

Default: <*optional*> []

Label of the region where to set fields.

`rid` = <*Integer [0,]*>

Default: <*optional*> []

ID of the region where to set fields.

`time` = <*Double [0,]*>

Default: 0.0 []

Apply field setting in this record after this time. These times has to form an increasing sequence.

`init_conc` = <*abstract type: Field:R3 → Real[n]*>

Default: <*optional*> []

Initial concentrations.

`por_m` = <*abstract type: Field:R3 → Real*>

Default: <*optional*> []

Mobile porosity

`disp_l` = <*abstract type: Field:R3 → Real*>

Default: <*optional*> []

Longitudal dispersivity.

`disp_t` = <*abstract type: Field:R3 → Real*>

Default: <*optional*> []

Transversal dispersivity.

`diff_m` = <*abstract type: Field:R3 → Real*>

Default: <*optional*> []

Molecular diffusivity.

`sigma_c` = <*abstract type: Field:R3 → Real*>

Default: <*optional*> []

Coefficient of diffusive transfer through fractures.

`dg_penalty` = <*abstract type: Field:R3 → Real*>

Default: <*optional*> []

Penalty parameter influencing the discontinuity of the solution.

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