

Technical university of Liberec
Faculty of mechatronics, informatics
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Flow123d

version 1.8.JHy_python_update

Documentation of file formats
and brief user manual.

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record: **IT::Root**

Root record of JSON input for Flow123d.

Root::problem = \langle abstract type: *IT::Problem* \rangle

Default: \langle obligatory \rangle

Simulation problem to be solved.

Root::pause_after_run = \langle Bool \rangle

Default: false

If true, the program will wait for key press before it terminates.

abstract type: **IT::Problem**

Descendants:

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

IT::SequentialCoupling

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

Record with data for a general sequential coupling.

SequentialCoupling::TYPE = \langle selection: *Problem_TYPE_selection* \rangle

Default: SequentialCoupling

Sub-record selection.

SequentialCoupling::description = \langle String (generic) \rangle

Default: \langle optional \rangle

Short description of the solved problem.

Is displayed in the main log, and possibly in other text output files.

SequentialCoupling::mesh = \langle record: *IT::Mesh* \rangle

Default: \langle obligatory \rangle

Computational mesh common to all equations.

SequentialCoupling::time = \langle record: *IT::TimeGovernor* \rangle

Default: \langle optional \rangle

Simulation time frame and time step.

SequentialCoupling::primary_equation = \langle abstract type: *IT::DarcyFlowMH* \rangle

Default: \langle obligatory \rangle

Primary equation, have all data given.

SequentialCoupling::secondary_equation = \langle abstract type: *IT::Transport* \rangle

Default: \langle optional \rangle

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

record: **IT::Mesh**

Record with mesh related data.

Mesh::mesh_file = \langle input file name \rangle

Default: \langle obligatory \rangle

Input file with mesh description.

Mesh::regions = \langle Array of Record: *IT::Region* \rangle

Default: \langle optional \rangle

List of additional region definitions not contained in the mesh.

Mesh::sets = $\langle \text{Array of Record: } \textcolor{red}{IT::RegionSet} \rangle$
 Default: $\langle \text{optional} \rangle$
 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)

Mesh::partitioning = $\langle \text{record: } \textcolor{red}{IT::Partition} \rangle$
 Default: $\langle \text{any_neighboring} \rangle$
 Parameters of mesh partitioning algorithms.

record: **IT::Region**

Definition of region of elements.

Region::name = $\langle \text{String (generic)} \rangle$
 Default: $\langle \text{obligatory} \rangle$
 Label (name) of the region. Has to be unique in one mesh.

Region::id = $\langle \text{Integer}[0,] \rangle$
 Default: $\langle \text{obligatory} \rangle$
 The ID of the region to which you assign label.

Region::element_list = $\langle \text{Array of Integer } [0,] \rangle$
 Default: $\langle \text{optional} \rangle$
 Specification of the region by the list of elements. This is not recommended

record: **IT::RegionSet**

Definition of one region set.

RegionSet::name = $\langle \text{String (generic)} \rangle$
 Default: $\langle \text{obligatory} \rangle$
 Unique name of the region set.

RegionSet::region_ids = $\langle \text{Array of Integer } [0,] \rangle$
 Default: $\langle \text{optional} \rangle$
 List of region ID numbers that has to be added to the region set.

RegionSet::region_labels = $\langle \text{Array of String (generic)} \rangle$
 Default: $\langle \text{optional} \rangle$
 List of labels of the regions that has to be added to the region set.

RegionSet::union = $\langle \text{Array } [2, 2] \text{ of String (generic)} \rangle$
 Default: $\langle \text{optional} \rangle$
 Defines region set as a union of given pair of sets. Overrides previous keys.

RegionSet::intersection = $\langle \text{Array } [2, 2] \text{ of String (generic)} \rangle$
 Default: $\langle \text{optional} \rangle$
 Defines region set as an intersection of given pair of sets. Overrides previous keys.

RegionSet::difference = $\langle \text{Array } [2, 2] \text{ of String (generic)} \rangle$
 Default: $\langle \text{optional} \rangle$
 Defines region set as a difference of given pair of sets. Overrides previous keys.

record: **IT::Partition** constructible from key: $\textcolor{red}{Partition::graph_type}$

Setting for various types of mesh partitioning.

`Partition::tool = \langle selection: IT::PartTool \rangle`

Default: METIS

Software package used for partitioning. See corresponding selection.

`Partition::graph_type = \langle selection: IT::GraphType \rangle`

Default: any_neighboring

Algorithm for generating graph and its weights from a multidimensional mesh.

selection type: **IT::PartTool**

Select the partitioning tool to use.

Possible values:

PETSc : Use PETSc interface to various partitioning tools.

METIS : Use direct interface to Metis.

selection type: **IT::GraphType**

Different algorithms to make the sparse graph with weighted edges from the multidimensional mesh. Main difference is dealing with neighborings of elements of different dimension.

Possible values:

any_neighboring : Add edge for any pair of neighboring elements.

any_wight_lower_dim_cuts : Same as before and assign higher weight to cuts of lower dimension in order to make them stick to one face.

same_dimension_neighboring : Add edge for any pair of neighboring elements of same dimension (bad for matrix multiply).

record: **IT::TimeGovernor** constructible from key: *TimeGovernor::max_dt*

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

`TimeGovernor::start_time = \langle Double \rangle`

Default: $\langle 0.0 \rangle$

Start time of the simulation.

`TimeGovernor::end_time = \langle Double \rangle`

Default: Infinite end time.

End time of the simulation.

`TimeGovernor::init_dt = \langle Double[0,] \rangle`

Default: $\langle 0.0 \rangle$

Initial guess for the time step.

Only useful for equations that use adaptive time stepping. If set to 0.0, the time step is determined in fully autonomous way if the equation supports it.

`TimeGovernor::min_dt = \langle Double[0,] \rangle`

Default: Machine precision.

Soft lower limit for the time step. Equation using adaptive time stepping can not suggest smaller time step, but actual time step could be smaller in order to match prescribed input or output times.

`TimeGovernor::max_dt = \langle Double[0,] \rangle`

Default: Whole time of the simulation if specified, infinity else.

Hard upper limit for the time step. Actual length of the time step is also limited by input and output times.

abstract type: **IT::DarcyFlowMH**

Descendants:

Mixed-Hybrid solver for saturated Darcy flow.

IT::Steady_MH

IT::Unsteady_MH

IT::Unsteady_LMH

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

Mixed-Hybrid solver for STEADY saturated Darcy flow.

Steady_MH::TYPE = $\langle \text{selection: } \textit{DarcyFlowMH_TYPE_selection} \rangle$

Default: **Steady_MH**

Sub-record selection.

Steady_MH::n_schurs = $\langle \textit{Integer}[0, 2] \rangle$

Default: $\langle 2 \rangle$

Number of Schur complements to perform when solving MH sytem.

Steady_MH::solver = $\langle \text{abstract type: } \textit{IT::LinSys} \rangle$

Default: $\langle \textit{obligatory} \rangle$

Linear solver for MH problem.

Steady_MH::output = $\langle \text{record: } \textit{IT::DarcyMHOutput} \rangle$

Default: $\langle \textit{obligatory} \rangle$

Parameters of output form MH module.

Steady_MH::mortar_method = $\langle \text{selection: } \textit{IT::MH_MortarMethod} \rangle$

Default: **None**

Method for coupling Darcy flow between dimensions.

Steady_MH::balance = $\langle \text{record: } \textit{IT::Balance} \rangle$

Default: $\langle \textit{obligatory} \rangle$

Settings for computing mass balance.

Steady_MH::input_fields = $\langle \textit{Array of Record: } \textit{IT::DarcyFlowMH_Data} \rangle$

Default: $\langle \textit{obligatory} \rangle$

abstract type: **IT::LinSys**

Descendants:

Linear solver setting.

IT::Petsc

IT::Bddc

record: **IT::Petsc** implements abstract type: **IT::LinSys**

Solver setting.

Petsc::TYPE = $\langle \text{selection: } \textit{LinSys_TYPE_selection} \rangle$

Default: **Petsc**

Sub-record selection.

Petsc::r_tol = $\langle \textit{Double}[0, 1] \rangle$

Default: $\langle 1.0e-7 \rangle$

Relative residual tolerance (to initial error).

Petsc::max_it = $\langle \textit{Integer}[0,] \rangle$

Default: $\langle 10000 \rangle$
Maximum number of outer iterations of the linear solver.

Petsc::a_tol = $\langle \text{Double}[0,] \rangle$
Default: $\langle 1.0e-9 \rangle$
Absolute residual tolerance.

Petsc::options = $\langle \text{String (generic)} \rangle$
Default: $\langle \text{value at declaration} \rangle$
Options passed to PETSC before creating KSP instead of default setting.

record: **IT::Bddc** implements abstract type: **IT::LinSys**

Solver setting.

Bddc::TYPE = $\langle \text{selection: LinSys_TYPE_selection} \rangle$
Default: Bddc
Sub-record selection.

Bddc::r_tol = $\langle \text{Double}[0, 1] \rangle$
Default: $\langle 1.0e-7 \rangle$
Relative residual tolerance (to initial error).

Bddc::max_it = $\langle \text{Integer}[0,] \rangle$
Default: $\langle 10000 \rangle$
Maximum number of outer iterations of the linear solver.

Bddc::max_nondecr_it = $\langle \text{Integer}[0,] \rangle$
Default: $\langle 30 \rangle$
Maximum number of iterations of the linear solver with non-decreasing residual.

Bddc::number_of_levels = $\langle \text{Integer}[0,] \rangle$
Default: $\langle 2 \rangle$
Number of levels in the multilevel method (=2 for the standard BDDC).

Bddc::use_adaptive_bddc = $\langle \text{Bool} \rangle$
Default: false
Use adaptive selection of constraints in BDDCML.

Bddc::bddcml_verbosity_level = $\langle \text{Integer}[0, 2] \rangle$
Default: $\langle 0 \rangle$
Level of verbosity of the BDDCML library: 0 - no output, 1 - mild output, 2 - detailed output.

record: **IT::DarcyMHOutput**

Parameters of MH output.

DarcyMHOutput::output_stream = $\langle \text{record: IT::OutputStream} \rangle$
Default: $\langle \text{obligatory} \rangle$
Parameters of output stream.

DarcyMHOutput::output_fields = $\langle \text{Array of Selection: IT::DarcyMHOutput_Selection} \rangle$
Default: $\langle \text{obligatory} \rangle$
List of fields to write to output file.

DarcyMHOutput::compute_errors = $\langle \text{Bool} \rangle$
Default: false

SPECIAL PURPOSE. Computing errors pro non-compatible coupling.

DarcyMHOutput::raw_flow_output = $\langle output\ file\ name \rangle$

Default: $\langle optional \rangle$

Output file with raw data form MH module.

record: **IT::OutputStream**

Parameters of output.

OutputStream::file = $\langle output\ file\ name \rangle$

Default: $\langle obligatory \rangle$

File path to the connected output file.

OutputStream::format = $\langle abstract\ type: IT::OutputTime \rangle$

Default: $\langle optional \rangle$

Format of output stream and possible parameters.

OutputStream::time_step = $\langle Double[0,] \rangle$

Default: $\langle optional \rangle$

Time interval between outputs.

Regular grid of output time points starts at the initial time of the equation and ends at the end time which must be specified.

The start time and the end time are always added.

OutputStream::time_list = $\langle Array\ of\ Double \rangle$

Default: List containing the initial time of the equation. You can prescribe an empty list to override this behavior.

Explicit array of output time points (can be combined with 'time_step'.

OutputStream::add_input_times = $\langle Bool \rangle$

Default: false

Add all input time points of the equation, mentioned in the 'input_fields' list, also as the output points.

abstract type: **IT::OutputTime**

Descendants:

Format of output stream and possible parameters.

IT::vtk

IT::gmsh

record: **IT::vtk** implements abstract type: **IT::OutputTime**

Parameters of vtk output format.

vtk::TYPE = $\langle selection: OutputTime_TYPE_selection \rangle$

Default: vtk

Sub-record selection.

vtk::variant = $\langle selection: IT::VTK\ variant\ (ascii\ or\ binary) \rangle$

Default: ascii

Variant of output stream file format.

vtk::parallel = $\langle Bool \rangle$

Default: false

Parallel or serial version of file format.

vtk::compression = $\langle selection: IT::Type\ of\ compression\ of\ VTK\ file\ format \rangle$

Default: none

Compression used in output stream file format.

selection type: **IT::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: **IT::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: **IT::gmsh** implements abstract type: **IT::OutputTime**

Parameters of gmsh output format.

gmsh::TYPE = $\langle selection: OutputTime_TYPE_selection \rangle$

Default: gmsh

Sub-record selection.

selection type: **IT::DarcyMHOutput_Selection**

Selection of fields available for output.

Possible values:

anisotropy : Output of the field anisotropy $[-]$ (Anisotropy of the conductivity tensor.).

cross_section : Output of the field cross_section $[m^{3-d}]$ (Complement dimension parameter (cross section for 1D, thickness for 2D).).

conductivity : Output of the field conductivity $[ms^{-1}]$ (Isotropic conductivity scalar.).

sigma : Output of the field sigma $[-]$ (Transition coefficient between dimensions.).

water_source_density : Output of the field water_source_density $[s^{-1}]$ (Water source density.).

init_pressure : Output of the field init_pressure $[m]$ (Initial condition as pressure).

storativity : Output of the field storativity $[m^{-1}]$ (Storativity.).

pressure_p0 : Output of the field pressure_p0 $[m]$.

pressure_p1 : Output of the field pressure_p1 $[m]$.

piezo_head_p0 : Output of the field piezo_head_p0 $[m]$.

velocity_p0 : Output of the field velocity_p0 $[ms^{-1}]$.

subdomain : Output of the field subdomain $[-]$.

region_id : Output of the field region_id $[-]$.

pressure_diff : Output of the field pressure_diff $[m]$.

velocity_diff : Output of the field velocity_diff $[ms^{-1}]$.

div_diff : Output of the field div_diff $[s^{-1}]$.

selection type: **IT::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: **IT::Balance** constructible from key: **Balance::balance_on**

Balance of a conservative quantity, boundary fluxes and sources.

Balance::balance_on = $\langle Bool \rangle$

Default: true

Balance is computed if the value is true.

Balance::format = $\langle selection: IT::Balance_output_format \rangle$

Default: txt

Format of output file.

Balance::cumulative = $\langle Bool \rangle$

Default: false

Compute cumulative balance over time. If true, then balance is calculated at each computational time step, which can slow down the program.

Balance::file = $\langle output\ file\ name \rangle$

Default: FileName balance.*

File name for output of balance.

selection type: **IT::Balance_output_format**

Format of output file for balance.

Possible values:

legacy : Legacy format used by previous program versions.

txt : Excel format with tab delimiter.

gnuplot : Format compatible with GnuPlot datafile with fixed column width.

record: **IT::DarcyFlowMH_Data**

Record to set fields of the equation.

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_Data record that comes later in the boundary data array.

DarcyFlowMH_Data::r_set = $\langle String\ (generic) \rangle$

Default: $\langle optional \rangle$

Name of region set where to set fields.

DarcyFlowMH_Data::region = $\langle String\ (generic) \rangle$

Default: $\langle optional \rangle$

Label of the region where to set fields.

DarcyFlowMH_Data::rid = $\langle Integer[0,] \rangle$

Default: $\langle optional \rangle$

ID of the region where to set fields.

DarcyFlowMH_Data::time = $\langle Double[0,] \rangle$

Default: $\langle 0.0 \rangle$

Apply field setting in this record after this time.

These times have to form an increasing sequence.

`DarcyFlowMH_Data::anisotropy` = $\langle \text{abstract type: } IT::Field:R3 \rightarrow Real[3,3] \rangle$
 Default: $\langle optional \rangle$
 Anisotropy of the conductivity tensor. $[-]$

`DarcyFlowMH_Data::cross_section` = $\langle \text{abstract type: } IT::Field:R3 \rightarrow Real \rangle$
 Default: $\langle optional \rangle$
 Complement dimension parameter (cross section for 1D, thickness for 2D).
 $[m^{3-d}]$

`DarcyFlowMH_Data::conductivity` = $\langle \text{abstract type: } IT::Field:R3 \rightarrow Real \rangle$
 Default: $\langle optional \rangle$
 Isotropic conductivity scalar. $[ms^{-1}]$

`DarcyFlowMH_Data::sigma` = $\langle \text{abstract type: } IT::Field:R3 \rightarrow Real \rangle$
 Default: $\langle optional \rangle$
 Transition coefficient between dimensions. $[-]$

`DarcyFlowMH_Data::water_source_density` = $\langle \text{abstract type: } IT::Field:R3 \rightarrow Real \rangle$
 Default: $\langle optional \rangle$
 Water source density. $[s^{-1}]$

`DarcyFlowMH_Data::bc_type` = $\langle \text{abstract type: } IT::Field:R3 \rightarrow Enum \rangle$
 Default: $\langle optional \rangle$
 Boundary condition type, possible values: $[-]$

`DarcyFlowMH_Data::bc_pressure` = $\langle \text{abstract type: } IT::Field:R3 \rightarrow Real \rangle$
 Default: $\langle optional \rangle$
 Dirichlet BC condition value for pressure. $[m]$

`DarcyFlowMH_Data::bc_flux` = $\langle \text{abstract type: } IT::Field:R3 \rightarrow Real \rangle$
 Default: $\langle optional \rangle$
 Flux in Neumann or Robin boundary condition. $[m^{4-d}s^{-1}]$

`DarcyFlowMH_Data::bc_robin_sigma` = $\langle \text{abstract type: } IT::Field:R3 \rightarrow Real \rangle$
 Default: $\langle optional \rangle$
 Conductivity coefficient in Robin boundary condition. $[m^{3-d}s^{-1}]$

`DarcyFlowMH_Data::init_pressure` = $\langle \text{abstract type: } IT::Field:R3 \rightarrow Real \rangle$
 Default: $\langle optional \rangle$
 Initial condition as pressure $[m]$

`DarcyFlowMH_Data::storativity` = $\langle \text{abstract type: } IT::Field:R3 \rightarrow Real \rangle$
 Default: $\langle optional \rangle$
 Storativity. $[m^{-1}]$

`DarcyFlowMH_Data::bc_piezo_head` = $\langle \text{abstract type: } IT::Field:R3 \rightarrow Real \rangle$
 Default: $\langle optional \rangle$
 Boundary condition for pressure as piezometric head.

`DarcyFlowMH_Data::init_piezo_head` = $\langle \text{abstract type: } IT::Field:R3 \rightarrow Real \rangle$
 Default: $\langle optional \rangle$
 Initial condition for pressure as piezometric head.

`DarcyFlowMH_Data::flow_old_bcd_file` = $\langle \text{input file name} \rangle$
 Default: $\langle optional \rangle$
 File with mesh dependent boundary conditions (obsolete).

abstract type: **`IT::Field:R3`** \rightarrow **`Real[3,3]`** default descendant: **`IT::FieldConstant`**

Descendants:

Abstract record for all time-space functions.

IT::FieldConstant

IT::FieldPython

IT::FieldFormula

IT::FieldElementwise

IT::FieldInterpolatedP0

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

R3 \rightarrow Real[3,3] Field constant in space.

FieldConstant::TYPE = $\langle \text{selection: Field:R3} \rightarrow \text{Real[3,3]}_TYPE_selection \rangle$

Default: FieldConstant

Sub-record selection.

FieldConstant::value = $\langle \text{Array [1,] of Array} \rangle$

Default: $\langle \text{obligatory} \rangle$

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: **IT::FieldPython** implements abstract type: **IT::Field:R3 \rightarrow Real[3,3]**

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

FieldPython::TYPE = $\langle \text{selection: Field:R3} \rightarrow \text{Real[3,3]}_TYPE_selection \rangle$

Default: FieldPython

Sub-record selection.

FieldPython::script_string = $\langle \text{String (generic)} \rangle$

Default: $\langle \text{value at read time} \rangle$

Python script given as in place string

FieldPython::script_file = $\langle \text{input file name} \rangle$

Default: Obligatory if 'script_striong' is not given.

Python script given as external file

FieldPython::function = $\langle \text{String (generic)} \rangle$

Default: $\langle \text{obligatory} \rangle$

Function in the given script that returns tuple containing components of the return type.

For NxM tensor values: $\text{tensor}(\text{row}, \text{col}) = \text{tuple}(M * \text{row} + \text{col})$.

record: **IT::FieldFormula** implements abstract type: **IT::Field:R3 \rightarrow Real[3,3]**

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

FieldFormula::TYPE = $\langle \text{selection: Field:R3} \rightarrow \text{Real[3,3]}_TYPE_selection \rangle$

Default: FieldFormula

Sub-record selection.

FieldFormula::value = $\langle \text{Array [1,] of Array} \rangle$

Default: $\langle \text{obligatory} \rangle$

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: **IT::FieldElementwise** implements abstract type: **IT::Field:R3 \rightarrow Real[3,3]**

R3 \rightarrow Real[3,3] Field constant in space.

FieldElementwise::TYPE = $\langle selection: Field:R3 \rightarrow Real[3,3]_{TYPE_selection} \rangle$

Default: FieldElementwise

Sub-record selection.

FieldElementwise::gmsh_file = $\langle input\ file\ name \rangle$

Default: $\langle obligatory \rangle$

Input file with ASCII GMSH file format.

FieldElementwise::field_name = $\langle String\ (generic) \rangle$

Default: $\langle obligatory \rangle$

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

record: **IT::FieldInterpolatedP0** implements abstract type: **IT::Field:R3 \rightarrow Real[3,3]**

R3 \rightarrow Real[3,3] Field constant in space.

FieldInterpolatedP0::TYPE = $\langle selection: Field:R3 \rightarrow Real[3,3]_{TYPE_selection} \rangle$

Default: FieldInterpolatedP0

Sub-record selection.

FieldInterpolatedP0::gmsh_file = $\langle input\ file\ name \rangle$

Default: $\langle obligatory \rangle$

Input file with ASCII GMSH file format.

FieldInterpolatedP0::field_name = $\langle String\ (generic) \rangle$

Default: $\langle obligatory \rangle$

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

abstract type: **IT::Field:R3 \rightarrow Real** default descendant: **IT::FieldConstant**

Descendants:

Abstract record for all time-space functions.

IT::FieldConstant

IT::FieldPython

IT::FieldFormula

IT::FieldElementwise

IT::FieldInterpolatedP0

record: **IT::FieldConstant** implements abstract type: **IT::Field:R3 \rightarrow Real** constructible from key: **FieldConstant::value**

R3 \rightarrow Real Field constant in space.

FieldConstant::TYPE = $\langle selection: Field:R3 \rightarrow Real_TYPE_selection \rangle$

Default: FieldConstant

Sub-record selection.

FieldConstant::value = $\langle Double \rangle$

Default: $\langle obligatory \rangle$

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: **IT::FieldPython** implements abstract type: **IT::Field:R3 \rightarrow Real**

R3 \rightarrow Real Field given by a Python script.

FieldPython::TYPE = $\langle selection: Field:R3 \rightarrow Real_TYPE_selection \rangle$

Default: FieldPython

Sub-record selection.

FieldPython::script_string = $\langle String (generic) \rangle$

Default: $\langle value\ at\ read\ time \rangle$

Python script given as in place string

FieldPython::script_file = $\langle input\ file\ name \rangle$

Default: Obligatory if 'script_string' is not given.

Python script given as external file

FieldPython::function = $\langle String (generic) \rangle$

Default: $\langle obligatory \rangle$

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: **IT::FieldFormula** implements abstract type: **IT::Field:R3 \rightarrow Real**

R3 \rightarrow Real Field given by runtime interpreted formula.

FieldFormula::TYPE = $\langle selection: Field:R3 \rightarrow Real_TYPE_selection \rangle$

Default: FieldFormula

Sub-record selection.

FieldFormula::value = $\langle String (generic) \rangle$

Default: $\langle obligatory \rangle$

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

R3 → Real Field constant in space.

FieldElementwise::TYPE = $\langle selection: Field:R3 \rightarrow Real_TYPE_selection \rangle$
Default: FieldElementwise
Sub-record selection.

FieldElementwise::gmsh_file = $\langle input\ file\ name \rangle$
Default: $\langle obligatory \rangle$
Input file with ASCII GMSH file format.

FieldElementwise::field_name = $\langle String\ (generic) \rangle$
Default: $\langle obligatory \rangle$
The values of the Field are read from the \$ElementData section with field name given by this key.

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

R3 → Real Field constant in space.

FieldInterpolatedP0::TYPE = $\langle selection: Field:R3 \rightarrow Real_TYPE_selection \rangle$
Default: FieldInterpolatedP0
Sub-record selection.

FieldInterpolatedP0::gmsh_file = $\langle input\ file\ name \rangle$
Default: $\langle obligatory \rangle$
Input file with ASCII GMSH file format.

FieldInterpolatedP0::field_name = $\langle String\ (generic) \rangle$
Default: $\langle obligatory \rangle$
The values of the Field are read from the \$ElementData section with field name given by this key.

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

Descendants:

Abstract record for all time-space functions.

IT::FieldConstant

IT::FieldFormula

IT::FieldPython

IT::FieldInterpolatedP0

IT::FieldElementwise

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

R3 → Enum Field constant in space.

FieldConstant::TYPE = $\langle selection: Field:R3 \rightarrow Enum_TYPE_selection \rangle$
Default: FieldConstant
Sub-record selection.

FieldConstant::value = $\langle \text{selection: } \textcolor{red}{IT::DarcyFlow_BC_Type} \rangle$

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: **IT::DarcyFlow_BC_Type**

Possible values:

none : Homogeneous Neumann boundary condition. Zero flux

dirichlet : Dirichlet boundary condition. Specify the pressure head through the 'bc_pressure' field or the piezometric head through the 'bc_piezo_head' field.

neumann : Neumann boundary condition. Prescribe water outflow by the 'bc_flux' field.

robin : Robin boundary condition. Water outflow equal to $\sigma(h - h^R)$. Specify the transition coefficient by 'bc_sigma' and the reference pressure head or piezometric head through 'bc_pressure' and 'bc_piezo_head' respectively.

record: **IT::FieldFormula** implements abstract type: $\textcolor{red}{IT::Field:R3 \rightarrow Enum}$

R3 \rightarrow Enum Field given by runtime interpreted formula.

FieldFormula::TYPE = $\langle \text{selection: } \textit{Field:R3} \rightarrow \textit{Enum_TYPE_selection} \rangle$

Default: FieldFormula

Sub-record selection.

FieldFormula::value = $\langle \textit{String (generic)} \rangle$

Default: $\langle \textit{obligatory} \rangle$

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: **IT::FieldPython** implements abstract type: $\textcolor{red}{IT::Field:R3 \rightarrow Enum}$

R3 \rightarrow Enum Field given by a Python script.

FieldPython::TYPE = $\langle \text{selection: } \textit{Field:R3} \rightarrow \textit{Enum_TYPE_selection} \rangle$

Default: FieldPython

Sub-record selection.

FieldPython::script_string = $\langle \textit{String (generic)} \rangle$

Default: $\langle \textit{value at read time} \rangle$

Python script given as in place string

FieldPython::script_file = $\langle \textit{input file name} \rangle$

Default: Obligatory if 'script_string' is not given.

Python script given as external file
FieldPython::function = $\langle \text{String (generic)} \rangle$
 Default: $\langle \text{obligatory} \rangle$
 Function in the given script that returns tuple containing components of the return type.
 For NxM tensor values: $\text{tensor}(\text{row}, \text{col}) = \text{tuple}(M * \text{row} + \text{col})$.

record: **IT::FieldInterpolatedP0** implements abstract type: **IT::Field:R3 \rightarrow Enum**

R3 \rightarrow Enum Field constant in space.

FieldInterpolatedP0::TYPE = $\langle \text{selection: Field:R3} \rightarrow \text{Enum_TYPE_selection} \rangle$

Default: FieldInterpolatedP0

Sub-record selection.

FieldInterpolatedP0::gmsh_file = $\langle \text{input file name} \rangle$

Default: $\langle \text{obligatory} \rangle$

Input file with ASCII GMSH file format.

FieldInterpolatedP0::field_name = $\langle \text{String (generic)} \rangle$

Default: $\langle \text{obligatory} \rangle$

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

record: **IT::FieldElementwise** implements abstract type: **IT::Field:R3 \rightarrow Enum**

R3 \rightarrow Enum Field constant in space.

FieldElementwise::TYPE = $\langle \text{selection: Field:R3} \rightarrow \text{Enum_TYPE_selection} \rangle$

Default: FieldElementwise

Sub-record selection.

FieldElementwise::gmsh_file = $\langle \text{input file name} \rangle$

Default: $\langle \text{obligatory} \rangle$

Input file with ASCII GMSH file format.

FieldElementwise::field_name = $\langle \text{String (generic)} \rangle$

Default: $\langle \text{obligatory} \rangle$

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

abstract type: **IT::Field:R3 \rightarrow Real** default descendant: **IT::FieldConstant**

Descendants:

Abstract record for all time-space functions.

IT::FieldConstant

IT::FieldFormula

IT::FieldPython

IT::FieldInterpolatedP0

IT::FieldElementwise

record: **IT::FieldConstant** implements abstract type: **IT::Field:R3 \rightarrow Real** constructible from key: **FieldConstant::value**

R3 \rightarrow Real Field constant in space.

FieldConstant::TYPE = $\langle selection: Field:R3 \rightarrow Real_TYPE_selection \rangle$

Default: FieldConstant

Sub-record selection.

FieldConstant::value = $\langle Double \rangle$

Default: $\langle obligatory \rangle$

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: **IT::FieldFormula** implements abstract type: **IT::Field:R3 \rightarrow Real**

R3 \rightarrow Real Field given by runtime interpreted formula.

FieldFormula::TYPE = $\langle selection: Field:R3 \rightarrow Real_TYPE_selection \rangle$

Default: FieldFormula

Sub-record selection.

FieldFormula::value = $\langle String (generic) \rangle$

Default: $\langle obligatory \rangle$

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: **IT::FieldPython** implements abstract type: **IT::Field:R3 \rightarrow Real**

R3 \rightarrow Real Field given by a Python script.

FieldPython::TYPE = $\langle selection: Field:R3 \rightarrow Real_TYPE_selection \rangle$

Default: FieldPython

Sub-record selection.

FieldPython::script_string = $\langle String (generic) \rangle$

Default: $\langle value \text{ at read time } \rangle$

Python script given as in place string

FieldPython::script_file = $\langle input \text{ file name } \rangle$

Default: Obligatory if 'script_string' is not given.

Python script given as external file

FieldPython::function = $\langle String (generic) \rangle$

Default: $\langle obligatory \rangle$

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

R3 → Real Field constant in space.

FieldInterpolatedP0::TYPE = $\langle \text{selection: Field:R3} \rightarrow \text{Real_TYPE_selection} \rangle$

Default: FieldInterpolatedP0

Sub-record selection.

FieldInterpolatedP0::gmsh_file = $\langle \text{input file name} \rangle$

Default: $\langle \text{obligatory} \rangle$

Input file with ASCII GMSH file format.

FieldInterpolatedP0::field_name = $\langle \text{String (generic)} \rangle$

Default: $\langle \text{obligatory} \rangle$

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

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

R3 → Real Field constant in space.

FieldElementwise::TYPE = $\langle \text{selection: Field:R3} \rightarrow \text{Real_TYPE_selection} \rangle$

Default: FieldElementwise

Sub-record selection.

FieldElementwise::gmsh_file = $\langle \text{input file name} \rangle$

Default: $\langle \text{obligatory} \rangle$

Input file with ASCII GMSH file format.

FieldElementwise::field_name = $\langle \text{String (generic)} \rangle$

Default: $\langle \text{obligatory} \rangle$

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

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

Descendants:

Abstract record for all time-space functions.

IT::FieldConstant

IT::FieldFormula

IT::FieldPython

IT::FieldInterpolatedP0

IT::FieldElementwise

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

Mixed-Hybrid solver for unsteady saturated Darcy flow.

Unsteady_MH::TYPE = $\langle \text{selection: DarcyFlowMH_TYPE_selection} \rangle$

Default: Unsteady_MH

Sub-record selection.

Unsteady_MH::n_schurs = $\langle \text{Integer}[0, 2] \rangle$

Default: $\langle 2 \rangle$

Number of Schur complements to perform when solving MH sytem.

Unsteady_MH::solver = $\langle \text{abstract type: IT::LinSys} \rangle$

Default: $\langle \text{obligatory} \rangle$

Linear solver for MH problem.

Unsteady_MH::output = $\langle \text{record: } \textcolor{red}{IT::DarcyMHOutput} \rangle$
 Default: $\langle \text{obligatory} \rangle$
 Parameters of output form MH module.

Unsteady_MH::mortar_method = $\langle \text{selection: } \textcolor{red}{IT::MH_MortarMethod} \rangle$
 Default: None
 Method for coupling Darcy flow between dimensions.

Unsteady_MH::balance = $\langle \text{record: } \textcolor{red}{IT::Balance} \rangle$
 Default: $\langle \text{obligatory} \rangle$
 Settings for computing mass balance.

Unsteady_MH::input_fields = $\langle \text{Array of Record: } \textcolor{red}{IT::DarcyFlowMH_Data} \rangle$
 Default: $\langle \text{obligatory} \rangle$

Unsteady_MH::time = $\langle \text{record: } \textcolor{red}{IT::TimeGovernor} \rangle$
 Default: $\langle \text{obligatory} \rangle$
 Time governor setting for the unsteady Darcy flow model.

record: **IT::Unsteady_LMH** implements abstract type: $\textcolor{red}{IT::DarcyFlowMH}$

Lumped Mixed-Hybrid solver for unsteady saturated Darcy flow.

Unsteady_LMH::TYPE = $\langle \text{selection: } \textcolor{red}{DarcyFlowMH_TYPE_selection} \rangle$
 Default: Unsteady_LMH
 Sub-record selection.

Unsteady_LMH::n_schurs = $\langle \text{Integer}[0, 2] \rangle$
 Default: $\langle 2 \rangle$
 Number of Schur complements to perform when solving MH sytem.

Unsteady_LMH::solver = $\langle \text{abstract type: } \textcolor{red}{IT::LinSys} \rangle$
 Default: $\langle \text{obligatory} \rangle$
 Linear solver for MH problem.

Unsteady_LMH::output = $\langle \text{record: } \textcolor{red}{IT::DarcyMHOutput} \rangle$
 Default: $\langle \text{obligatory} \rangle$
 Parameters of output form MH module.

Unsteady_LMH::mortar_method = $\langle \text{selection: } \textcolor{red}{IT::MH_MortarMethod} \rangle$
 Default: None
 Method for coupling Darcy flow between dimensions.

Unsteady_LMH::balance = $\langle \text{record: } \textcolor{red}{IT::Balance} \rangle$
 Default: $\langle \text{obligatory} \rangle$
 Settings for computing mass balance.

Unsteady_LMH::input_fields = $\langle \text{Array of Record: } \textcolor{red}{IT::DarcyFlowMH_Data} \rangle$
 Default: $\langle \text{obligatory} \rangle$

Unsteady_LMH::time = $\langle \text{record: } \textcolor{red}{IT::TimeGovernor} \rangle$
 Default: $\langle \text{obligatory} \rangle$
 Time governor setting for the unsteady Darcy flow model.

abstract type: **IT::Transport**

Descendants:

Secondary equation for transport of substances.

$\textcolor{red}{IT::TransportOperatorSplitting}$

$\textcolor{red}{IT::SoluteTransport_DG}$

IT::HeatTransfer_DG

record: **IT::TransportOperatorSplitting** implements abstract type: **IT::Transport**

Explicit FVM transport (no diffusion)
coupled with reaction and adsorption model (ODE per element)
via operator splitting.

TransportOperatorSplitting::TYPE = $\langle \textit{selection: Transport_TYPE_selection} \rangle$
Default: **TransportOperatorSplitting**
Sub-record selection.

TransportOperatorSplitting::time = $\langle \textit{record: IT::TimeGovernor} \rangle$
Default: $\langle \textit{obligatory} \rangle$
Time governor setting for the secondary equation.

TransportOperatorSplitting::balance = $\langle \textit{record: IT::Balance} \rangle$
Default: $\langle \textit{obligatory} \rangle$
Settings for computing balance.

TransportOperatorSplitting::output_stream = $\langle \textit{record: IT::OutputStream} \rangle$
Default: $\langle \textit{obligatory} \rangle$
Parameters of output stream.

TransportOperatorSplitting::substances = $\langle \textit{Array of Record: IT::Substance} \rangle$
Default: $\langle \textit{obligatory} \rangle$
Specification of transported substances.

TransportOperatorSplitting::reaction_term = $\langle \textit{abstract type: IT::ReactionTerm} \rangle$
Default: $\langle \textit{optional} \rangle$
Reaction model involved in transport.

TransportOperatorSplitting::input_fields = $\langle \textit{Array of Record: IT::TransportOperatorSplitting_Data} \rangle$
Default: $\langle \textit{obligatory} \rangle$

TransportOperatorSplitting::output_fields = $\langle \textit{Array of Selection: IT::ConvectionTransport_Output} \rangle$
Default: $\langle \textit{conc} \rangle$
List of fields to write to output file.

record: **IT::Substance** constructible from key: **Substance::name**

Chemical substance.

Substance::name = $\langle \textit{String (generic)} \rangle$
Default: $\langle \textit{obligatory} \rangle$
Name of the substance.

Substance::molar_mass = $\langle \textit{Double}[0,] \rangle$
Default: $\langle 1 \rangle$
Molar mass of the substance [kg/mol].

abstract type: **IT::ReactionTerm**

Descendants:

Equation for reading information about simple chemical reactions.

IT::FirstOrderReaction

IT::RadioactiveDecay

IT::Sorption
IT::SorptionMobile
IT::SorptionImmobile
IT::DualPorosity
IT::Semchem

record: **IT::FirstOrderReaction** implements abstract type: **IT::ReactionTerm**

A model of first order chemical reactions (decompositions of a reactant into products).

FirstOrderReaction::TYPE = $\langle \text{selection: ReactionTerm_TYPE_selection} \rangle$

Default: FirstOrderReaction

Sub-record selection.

FirstOrderReaction::reactions = $\langle \text{Array of Record: IT::Reaction} \rangle$

Default: $\langle \text{obligatory} \rangle$

An array of first order chemical reactions.

FirstOrderReaction::ode_solver = $\langle \text{abstract type: IT::LinearODESolver} \rangle$

Default: $\langle \text{optional} \rangle$

Numerical solver for the system of first order ordinary differential equations coming from the model.

record: **IT::Reaction**

Describes a single first order chemical reaction.

Reaction::reactants = $\langle \text{Array [1,] of Record: IT::FirstOrderReactionReactant} \rangle$

Default: $\langle \text{obligatory} \rangle$

An array of reactants. Do not use array, reactions with only one reactant (decays) are implemented at the moment!

Reaction::reaction_rate = $\langle \text{Double[0,]} \rangle$

Default: $\langle \text{obligatory} \rangle$

The reaction rate coefficient of the first order reaction.

Reaction::products = $\langle \text{Array [1,] of Record: IT::FirstOrderReactionProduct} \rangle$

Default: $\langle \text{obligatory} \rangle$

An array of products.

record: **IT::FirstOrderReactionReactant** constructible from key: **FirstOrderReactionReactant::name**

A record describing a reactant of a reaction.

FirstOrderReactionReactant::name = $\langle \text{String (generic)} \rangle$

Default: $\langle \text{obligatory} \rangle$

The name of the reactant.

record: **IT::FirstOrderReactionProduct** constructible from key: **FirstOrderReactionProduct::name**

A record describing a product of a reaction.

FirstOrderReactionProduct::name = $\langle \text{String (generic)} \rangle$

Default: $\langle \text{obligatory} \rangle$

The name of the product.

FirstOrderReactionProduct::branching_ratio = $\langle \text{Double}[0,] \rangle$

Default: $\langle 1.0 \rangle$

The branching ratio of the product when there are more products.

The value must be positive. Further, the branching ratios of all products are normalized in order to sum to one.

The default value 1.0, should only be used in the case of single product.

abstract type: **IT::LinearODESolver**

Descendants:

Solver of a linear system of ODEs.

IT::PadeApproximant

IT::LinearODEAnalytic

record: **IT::PadeApproximant** implements abstract type: **IT::LinearODESolver**

Record with an information about pade approximant parameters.

PadeApproximant::TYPE = $\langle \text{selection: LinearODESolver_TYPE_selection} \rangle$

Default: PadeApproximant

Sub-record selection.

PadeApproximant::nominator_degree = $\langle \text{Integer}[1,] \rangle$

Default: $\langle 2 \rangle$

Polynomial degree of the nominator of Pade approximant.

PadeApproximant::denominator_degree = $\langle \text{Integer}[1,] \rangle$

Default: $\langle 2 \rangle$

Polynomial degree of the denominator of Pade approximant

record: **IT::LinearODEAnalytic** implements abstract type: **IT::LinearODESolver**

Evaluate analytic solution of the system of ODEs.

LinearODEAnalytic::TYPE = $\langle \text{selection: LinearODESolver_TYPE_selection} \rangle$

Default: LinearODEAnalytic

Sub-record selection.

record: **IT::RadioactiveDecay** implements abstract type: **IT::ReactionTerm**

A model of a radioactive decay and possibly of a decay chain.

RadioactiveDecay::TYPE = $\langle \text{selection: ReactionTerm_TYPE_selection} \rangle$

Default: RadioactiveDecay

Sub-record selection.

RadioactiveDecay::decays = $\langle \text{Array}[1,] \text{ of Record: IT::Decay} \rangle$

Default: $\langle \text{obligatory} \rangle$

An array of radioactive decays.

RadioactiveDecay::ode_solver = $\langle \text{abstract type: IT::LinearODESolver} \rangle$

Default: $\langle \text{optional} \rangle$

Numerical solver for the system of first order ordinary differential equations coming from the model.

record: **IT::Decay**

A model of a radioactive decay.

`Decay::radionuclide` = $\langle \text{String (generic)} \rangle$

Default: $\langle \text{obligatory} \rangle$

The name of the parent radionuclide.

`Decay::half_life` = $\langle \text{Double}[0,] \rangle$

Default: $\langle \text{obligatory} \rangle$

The half life of the parent radionuclide in seconds.

`Decay::products` = $\langle \text{Array}[1,] \text{ of Record: } \textcolor{red}{IT::RadioactiveDecayProduct} \rangle$

Default: $\langle \text{obligatory} \rangle$

An array of the decay products (daughters).

record: **IT::RadioactiveDecayProduct** constructible from key: **RadioactiveDecayProduct::name**

A record describing a product of a radioactive decay.

`RadioactiveDecayProduct::name` = $\langle \text{String (generic)} \rangle$

Default: $\langle \text{obligatory} \rangle$

The name of the product.

`RadioactiveDecayProduct::energy` = $\langle \text{Double}[0,] \rangle$

Default: $\langle 0.0 \rangle$

Not used at the moment! The released energy in MeV from the decay of the radionuclide into the product.

`RadioactiveDecayProduct::branching_ratio` = $\langle \text{Double}[0,] \rangle$

Default: $\langle 1.0 \rangle$

The branching ratio of the product when there is more than one. Considering only one product, the default ratio 1.0 is used. Its value must be positive. Further, the branching ratios of all products are normalized by their sum, so the sum then gives 1.0 (this also resolves possible rounding errors).

record: **IT::Sorption** implements abstract type: **IT::ReactionTerm**

Sorption model in the reaction term of transport.

`Sorption::TYPE` = $\langle \text{selection: ReactionTerm_TYPE_selection} \rangle$

Default: Sorption

Sub-record selection.

`Sorption::substances` = $\langle \text{Array}[1,] \text{ of String (generic)} \rangle$

Default: $\langle \text{obligatory} \rangle$

Names of the substances that take part in the sorption model.

`Sorption::solvent_density` = $\langle \text{Double}[0,] \rangle$

Default: $\langle 1.0 \rangle$

Density of the solvent.

`Sorption::substeps` = $\langle \text{Integer}[1,] \rangle$

Default: $\langle 1000 \rangle$

Number of equidistant substeps, molar mass and isotherm intersections

`Sorption::solubility` = $\langle \text{Array of Double} \rangle$

Default: $\langle \text{optional} \rangle$

Specifies solubility limits of all the sorbing species.

`Sorption::table_limits` = $\langle \text{Array of Double} \rangle$

Default: $\langle optional \rangle$
 Specifies highest aqueous concentration in interpolation table.

Sorption::input_fields = $\langle Array \text{ of } Record: IT::Sorption_Data \rangle$
 Default: $\langle obligatory \rangle$
 Contains region specific data necessary to construct isotherms.

Sorption::reaction_liquid = $\langle abstract \text{ type: } IT::ReactionTerm \rangle$
 Default: $\langle optional \rangle$
 Reaction model following the sorption in the liquid.

Sorption::reaction_solid = $\langle abstract \text{ type: } IT::ReactionTerm \rangle$
 Default: $\langle optional \rangle$
 Reaction model following the sorption in the solid.

Sorption::output_fields = $\langle Array \text{ of } Selection: IT::Sorption_Output \rangle$
 Default: $\langle conc_solid \rangle$
 List of fields to write to output stream.

record: **IT::Sorption_Data**

Record to set fields of the equation.
 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 Sorption_Data record that comes later in the boundary data array.

Sorption_Data::r_set = $\langle String \text{ (generic) } \rangle$
 Default: $\langle optional \rangle$
 Name of region set where to set fields.

Sorption_Data::region = $\langle String \text{ (generic) } \rangle$
 Default: $\langle optional \rangle$
 Label of the region where to set fields.

Sorption_Data::rid = $\langle Integer[0,] \rangle$
 Default: $\langle optional \rangle$
 ID of the region where to set fields.

Sorption_Data::time = $\langle Double[0,] \rangle$
 Default: $\langle 0.0 \rangle$
 Apply field setting in this record after this time.
 These times have to form an increasing sequence.

Sorption_Data::rock_density = $\langle abstract \text{ type: } IT::Field:R3 \rightarrow Real \rangle$
 Default: $\langle optional \rangle$
 Rock matrix density. $[m^{-3}kg]$

Sorption_Data::sorption_type = $\langle abstract \text{ type: } IT::Field:R3 \rightarrow Enum[n] \rangle$
 Default: $\langle optional \rangle$
 Considered sorption is described by selected isotherm. If porosity on an element is equal or even higher than 1.0 (meaning no sorbing surface), then type 'none' will be selected automatically. $[-]$

Sorption_Data::isotherm_mult = $\langle abstract \text{ type: } IT::Field:R3 \rightarrow Real[n] \rangle$
 Default: $\langle optional \rangle$

Multiplication parameters (k, omega) in either Langmuir $c_s = \omega * (\alpha * c_a) / (1 - \alpha * c_a)$ or in linear $c_s = k * c_a$ isothermal description. $[kg^{-1}mol]$

SorptionData::isotherm_other = $\langle \text{abstract type: } IT::Field:R3 \rightarrow Real[n] \rangle$
 Default: $\langle optional \rangle$
 Second parameters (alpha, ...) defining isotherm $c_s = \omega * (\alpha * c_a) / (1 - \alpha * c_a)$. $[-]$

SorptionData::init_conc_solid = $\langle \text{abstract type: } IT::Field:R3 \rightarrow Real[n] \rangle$
 Default: $\langle optional \rangle$
 Initial solid concentration of substances. Vector, one value for every substance. $[kg^{-1}mol]$

abstract type: **IT::Field:R3** \rightarrow **Enum[n]** default descendant: **IT::FieldConstant**

Descendants:

Abstract record for all time-space functions.

IT::FieldConstant

IT::FieldFormula

IT::FieldPython

IT::FieldInterpolatedP0

IT::FieldElementwise

record: **IT::FieldConstant** implements abstract type: **IT::Field:R3** \rightarrow **Enum[n]** constructible from key: **FieldConstant::value**

$R3 \rightarrow Enum[n]$ Field constant in space.

FieldConstant::TYPE = $\langle \text{selection: } Field:R3 \rightarrow Enum[n]_{TYPE_selection} \rangle$

Default: FieldConstant

Sub-record selection.

FieldConstant::value = $\langle \text{Array } [1,] \text{ of Selection: } IT::SorptionType \rangle$

Default: $\langle obligatory \rangle$

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: **IT::SorptionType**

Possible values:

none : No sorption considered.

linear : Linear isotherm runs the concentration exchange between liquid and solid.

langmuir : Langmuir isotherm runs the concentration exchange between liquid and solid.

freundlich : Freundlich isotherm runs the concentration exchange between liquid and solid.

record: **IT::FieldFormula** implements abstract type: **IT::Field:R3** \rightarrow **Enum[n]**

$R3 \rightarrow \text{Enum}[n]$ Field given by runtime interpreted formula.

FieldFormula::TYPE = $\langle \text{selection: Field:}R3 \rightarrow \text{Enum}[n]\text{-TYPE_selection} \rangle$
 Default: FieldFormula
 Sub-record selection.

FieldFormula::value = $\langle \text{Array } [1,] \text{ of String (generic)} \rangle$
 Default: $\langle \text{obligatory} \rangle$
 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: **IT::FieldPython** implements abstract type: **IT::Field:R3 \rightarrow Enum[n]**

$R3 \rightarrow \text{Enum}[n]$ Field given by a Python script.

FieldPython::TYPE = $\langle \text{selection: Field:}R3 \rightarrow \text{Enum}[n]\text{-TYPE_selection} \rangle$
 Default: FieldPython
 Sub-record selection.

FieldPython::script_string = $\langle \text{String (generic)} \rangle$
 Default: $\langle \text{value at read time} \rangle$
 Python script given as in place string

FieldPython::script_file = $\langle \text{input file name} \rangle$
 Default: Obligatory if 'script_string' is not given.
 Python script given as external file

FieldPython::function = $\langle \text{String (generic)} \rangle$
 Default: $\langle \text{obligatory} \rangle$
 Function in the given script that returns tuple containing components of the return type.
 For NxM tensor values: $\text{tensor}(\text{row}, \text{col}) = \text{tuple}(M * \text{row} + \text{col})$.

record: **IT::FieldInterpolatedP0** implements abstract type: **IT::Field:R3 \rightarrow Enum[n]**

$R3 \rightarrow \text{Enum}[n]$ Field constant in space.

FieldInterpolatedP0::TYPE = $\langle \text{selection: Field:}R3 \rightarrow \text{Enum}[n]\text{-TYPE_selection} \rangle$
 Default: FieldInterpolatedP0
 Sub-record selection.

FieldInterpolatedP0::gmsl_file = $\langle \text{input file name} \rangle$
 Default: $\langle \text{obligatory} \rangle$
 Input file with ASCII GMSH file format.

FieldInterpolatedP0::field_name = $\langle \text{String (generic)} \rangle$
 Default: $\langle \text{obligatory} \rangle$
 The values of the Field are read from the \$ElementData section with field name given by this key.

record: **IT::FieldElementwise** implements abstract type: **IT::Field:R3 \rightarrow Enum[n]**

R3 \rightarrow Enum[n] Field constant in space.

FieldElementwise::TYPE = $\langle selection: Field:R3 \rightarrow Enum[n]_{TYPE_selection} \rangle$
 Default: FieldElementwise
 Sub-record selection.

FieldElementwise::gmsh_file = $\langle input\ file\ name \rangle$
 Default: $\langle obligatory \rangle$
 Input file with ASCII GMSH file format.

FieldElementwise::field_name = $\langle String\ (generic) \rangle$
 Default: $\langle obligatory \rangle$
 The values of the Field are read from the \$ElementData section with field name given by this key.

abstract type: **IT::Field:R3 \rightarrow Real[n]** default descendant: **IT::FieldConstant**

Descendants:

Abstract record for all time-space functions.

IT::FieldConstant

IT::FieldPython

IT::FieldFormula

IT::FieldElementwise

IT::FieldInterpolatedP0

record: **IT::FieldConstant** implements abstract type: **IT::Field:R3 \rightarrow Real[n]** constructible from key: **FieldConstant::value**

R3 \rightarrow Real[n] Field constant in space.

FieldConstant::TYPE = $\langle selection: Field:R3 \rightarrow Real[n]_{TYPE_selection} \rangle$

Default: FieldConstant

Sub-record selection.

FieldConstant::value = $\langle Array\ [1,]\ of\ Double \rangle$

Default: $\langle obligatory \rangle$

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: **IT::FieldPython** implements abstract type: **IT::Field:R3 \rightarrow Real[n]**

R3 \rightarrow Real[n] Field given by a Python script.

FieldPython::TYPE = $\langle selection: Field:R3 \rightarrow Real[n]_{TYPE_selection} \rangle$

Default: FieldPython

Sub-record selection.

FieldPython::script_string = $\langle String\ (generic) \rangle$

Default: $\langle value\ at\ read\ time \rangle$

Python script given as in place string

FieldPython::script_file = $\langle \text{input file name} \rangle$
 Default: Obligatory if 'script_striong' is not given.
 Python script given as external file

FieldPython::function = $\langle \text{String (generic)} \rangle$
 Default: $\langle \text{obligatory} \rangle$
 Function in the given script that returns tuple containing components of the return type.
 For NxM tensor values: $\text{tensor}(\text{row}, \text{col}) = \text{tuple}(M * \text{row} + \text{col})$.

record: **IT::FieldFormula** implements abstract type: **IT::Field:R3 \rightarrow Real[n]**

R3 \rightarrow Real[n] Field given by runtime interpreted formula.

FieldFormula::TYPE = $\langle \text{selection: Field:R3} \rightarrow \text{Real[n]}_{\text{TYPE_selection}} \rangle$
 Default: FieldFormula
 Sub-record selection.

FieldFormula::value = $\langle \text{Array [1,] of String (generic)} \rangle$
 Default: $\langle \text{obligatory} \rangle$
 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: **IT::FieldElementwise** implements abstract type: **IT::Field:R3 \rightarrow Real[n]**

R3 \rightarrow Real[n] Field constant in space.

FieldElementwise::TYPE = $\langle \text{selection: Field:R3} \rightarrow \text{Real[n]}_{\text{TYPE_selection}} \rangle$
 Default: FieldElementwise
 Sub-record selection.

FieldElementwise::gmsb_file = $\langle \text{input file name} \rangle$
 Default: $\langle \text{obligatory} \rangle$
 Input file with ASCII GMSH file format.

FieldElementwise::field_name = $\langle \text{String (generic)} \rangle$
 Default: $\langle \text{obligatory} \rangle$
 The values of the Field are read from the \$ElementData section with field name given by this key.

record: **IT::FieldInterpolatedP0** implements abstract type: **IT::Field:R3 \rightarrow Real[n]**

R3 \rightarrow Real[n] Field constant in space.

FieldInterpolatedP0::TYPE = $\langle \text{selection: Field:R3} \rightarrow \text{Real[n]}_{\text{TYPE_selection}} \rangle$
 Default: FieldInterpolatedP0
 Sub-record selection.

FieldInterpolatedP0::gmsb_file = $\langle \text{input file name} \rangle$
 Default: $\langle \text{obligatory} \rangle$

Input file with ASCII GMSH file format.

FieldInterpolatedP0::field_name = $\langle \text{String (generic)} \rangle$

Default: $\langle \text{obligatory} \rangle$

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

selection type: **IT::Sorption_Output**

Possible values:

rock_density : Output of the field rock_density [$m^{-3}kg$] (Rock matrix density.).

sorption_type : Output of the field sorption_type $[-]$ (Considered sorption is described by selected isotherm. If porosity on an element is equal or even higher than 1.0 (meaning no sorbing surface), then type 'none' will be selected automatically.).

isotherm_mult : Output of the field isotherm_mult [$kg^{-1}mol$] (Multiplication parameters (k, omega) in either Langmuir $c_s = \omega * (\alpha * c_a) / (1 - \alpha * c_a)$ or in linear $c_s = k * c_a$ isothermal description.).

isotherm_other : Output of the field isotherm_other $[-]$ (Second parameters (alpha, ...) defining isotherm $c_s = \omega * (\alpha * c_a) / (1 - \alpha * c_a)$.).

init_conc_solid : Output of the field init_conc_solid [$kg^{-1}mol$] (Initial solid concentration of substances. Vector, one value for every substance.).

conc_solid : Output of the field conc_solid [$m^{-3}kg$].

record: **IT::SorptionMobile** implements abstract type: **IT::ReactionTerm**

Sorption model in the mobile zone, following the dual porosity model.

SorptionMobile::TYPE = $\langle \text{selection: ReactionTerm_TYPE_selection} \rangle$

Default: SorptionMobile

Sub-record selection.

SorptionMobile::substances = $\langle \text{Array [1,] of String (generic)} \rangle$

Default: $\langle \text{obligatory} \rangle$

Names of the substances that take part in the sorption model.

SorptionMobile::solvent_density = $\langle \text{Double}[0,] \rangle$

Default: $\langle 1.0 \rangle$

Density of the solvent.

SorptionMobile::substeps = $\langle \text{Integer}[1,] \rangle$

Default: $\langle 1000 \rangle$

Number of equidistant substeps, molar mass and isotherm intersections

SorptionMobile::solubility = $\langle \text{Array of Double} \rangle$

Default: $\langle \text{optional} \rangle$

Specifies solubility limits of all the sorbing species.

SorptionMobile::table_limits = $\langle \text{Array of Double} \rangle$

Default: $\langle \text{optional} \rangle$

Specifies highest aqueous concentration in interpolation table.

SorptionMobile::input_fields = $\langle \text{Array of Record: IT::Sorption_Data} \rangle$

Default: $\langle \text{obligatory} \rangle$

Contains region specific data necessary to construct isotherms.

SorptionMobile::reaction_liquid = $\langle \text{abstract type: IT::ReactionTerm} \rangle$

Default: $\langle \text{optional} \rangle$

Reaction model following the sorption in the liquid.

SorptionMobile::reaction_solid = $\langle \text{abstract type: } \textcolor{red}{IT::ReactionTerm} \rangle$

Default: $\langle \text{optional} \rangle$

Reaction model following the sorption in the solid.

SorptionMobile::output_fields = $\langle \text{Array of Selection: } \textcolor{red}{IT::SorptionMobile_Output} \rangle$

Default: $\langle \text{conc_solid} \rangle$

List of fields to write to output stream.

selection type: **IT::SorptionMobile_Output**

Possible values:

rock_density : Output of the field rock_density [$m^{-3}kg$] (Rock matrix density.).

sorption_type : Output of the field sorption_type $[-]$ (Considered sorption is described by selected isotherm. If porosity on an element is equal or even higher than 1.0 (meaning no sorbing surface), then type 'none' will be selected automatically.).

isotherm_mult : Output of the field isotherm_mult [$kg^{-1}mol$] (Multiplication parameters (k, omega) in either Langmuir $c_s = \omega * (\alpha * c_a) / (1 - \alpha * c_a)$ or in linear $c_s = k * c_a$ isothermal description.).

isotherm_other : Output of the field isotherm_other $[-]$ (Second parameters (alpha, ...) defining isotherm $c_s = \omega * (\alpha * c_a) / (1 - \alpha * c_a)$.).

init_conc_solid : Output of the field init_conc_solid [$kg^{-1}mol$] (Initial solid concentration of substances. Vector, one value for every substance.).

conc_solid : Output of the field conc_solid [$m^{-3}kg$].

record: **IT::SorptionImmobile** implements abstract type: $\textcolor{red}{IT::ReactionTerm}$

Sorption model in the immobile zone, following the dual porosity model.

SorptionImmobile::TYPE = $\langle \text{selection: } \text{ReactionTerm_TYPE_selection} \rangle$

Default: SorptionImmobile

Sub-record selection.

SorptionImmobile::substances = $\langle \text{Array } [1,] \text{ of String (generic)} \rangle$

Default: $\langle \text{obligatory} \rangle$

Names of the substances that take part in the sorption model.

SorptionImmobile::solvent_density = $\langle \text{Double}[0,] \rangle$

Default: $\langle 1.0 \rangle$

Density of the solvent.

SorptionImmobile::substeps = $\langle \text{Integer}[1,] \rangle$

Default: $\langle 1000 \rangle$

Number of equidistant substeps, molar mass and isotherm intersections

SorptionImmobile::solubility = $\langle \text{Array of Double} \rangle$

Default: $\langle \text{optional} \rangle$

Specifies solubility limits of all the sorbing species.

SorptionImmobile::table_limits = $\langle \text{Array of Double} \rangle$

Default: $\langle \text{optional} \rangle$

Specifies highest aqueous concentration in interpolation table.

SorptionImmobile::input_fields = $\langle \text{Array of Record: } \textcolor{red}{IT::Sorption_Data} \rangle$

Default: $\langle \text{obligatory} \rangle$

Contains region specific data necessary to construct isotherms.

SorptionImmobile::reaction_liquid = $\langle \text{abstract type: } \textcolor{red}{IT::ReactionTerm} \rangle$
 Default: $\langle \text{optional} \rangle$
 Reaction model following the sorption in the liquid.

SorptionImmobile::reaction_solid = $\langle \text{abstract type: } \textcolor{red}{IT::ReactionTerm} \rangle$
 Default: $\langle \text{optional} \rangle$
 Reaction model following the sorption in the solid.

SorptionImmobile::output_fields = $\langle \text{Array of Selection: } \textcolor{red}{IT::SorptionImmobile_Output} \rangle$
 Default: $\langle \text{conc_immobile_solid} \rangle$
 List of fields to write to output stream.

selection type: **IT::SorptionImmobile_Output**

Possible values:

rock_density: Output of the field rock_density [$m^{-3}kg$] (Rock matrix density.).

sorption_type: Output of the field sorption_type $[-]$ (Considered sorption is described by selected isotherm. If porosity on an element is equal or even higher than 1.0 (meaning no sorbing surface), then type 'none' will be selected automatically.).

isotherm_mult: Output of the field isotherm_mult [$kg^{-1}mol$] (Multiplication parameters (k, omega) in either Langmuir $c_s = \omega * (\alpha * c_a) / (1 - \alpha * c_a)$ or in linear $c_s = k * c_a$ isothermal description.).

isotherm_other: Output of the field isotherm_other $[-]$ (Second parameters (alpha, ...) defining isotherm $c_s = \omega * (\alpha * c_a) / (1 - \alpha * c_a)$.).

init_conc_solid: Output of the field init_conc_solid [$kg^{-1}mol$] (Initial solid concentration of substances. Vector, one value for every substance.).

conc_immobile_solid: Output of the field conc_immobile_solid [$m^{-3}kg$].

record: **IT::DualPorosity** implements abstract type: $\textcolor{red}{IT::ReactionTerm}$

Dual porosity model in transport problems.

Provides computing the concentration of substances in mobile and immobile zone.

DualPorosity::TYPE = $\langle \text{selection: } \text{ReactionTerm_TYPE_selection} \rangle$
 Default: DualPorosity
 Sub-record selection.

DualPorosity::input_fields = $\langle \text{Array of Record: } \textcolor{red}{IT::DualPorosity_Data} \rangle$
 Default: $\langle \text{obligatory} \rangle$
 Contains region specific data necessary to construct dual porosity model.

DualPorosity::scheme_tolerance = $\langle \text{Double}[0,] \rangle$
 Default: $\langle 1e-3 \rangle$
 Tolerance according to which the explicit Euler scheme is used or not. Set 0.0 to use analytic formula only (can be slower).

DualPorosity::reaction_mobile = $\langle \text{abstract type: } \textcolor{red}{IT::ReactionTerm} \rangle$
 Default: $\langle \text{optional} \rangle$
 Reaction model in mobile zone.

DualPorosity::reaction_immobile = $\langle \text{abstract type: } \textcolor{red}{IT::ReactionTerm} \rangle$
 Default: $\langle \text{optional} \rangle$
 Reaction model in immobile zone.

`DualPorosity::output_fields` = $\langle \text{Array of Selection: } \textcolor{red}{IT::DualPorosity_Output} \rangle$
 Default: $\langle \text{conc_immobile} \rangle$
 List of fields to write to output stream.

record: **IT::DualPorosity_Data**

Record to set fields of the equation.

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 `DualPorosity_Data` record that comes later in the boundary data array.

`DualPorosity_Data::r_set` = $\langle \text{String (generic)} \rangle$

Default: $\langle \text{optional} \rangle$

Name of region set where to set fields.

`DualPorosity_Data::region` = $\langle \text{String (generic)} \rangle$

Default: $\langle \text{optional} \rangle$

Label of the region where to set fields.

`DualPorosity_Data::rid` = $\langle \text{Integer}[0,] \rangle$

Default: $\langle \text{optional} \rangle$

ID of the region where to set fields.

`DualPorosity_Data::time` = $\langle \text{Double}[0,] \rangle$

Default: $\langle 0.0 \rangle$

Apply field setting in this record after this time.

These times have to form an increasing sequence.

`DualPorosity_Data::diffusion_rate_immobile` = $\langle \text{abstract type: } \textcolor{red}{IT::Field:R3} \rightarrow \textcolor{red}{Real}[n] \rangle$

Default: $\langle \text{optional} \rangle$

Diffusion coefficient of non-equilibrium linear exchange between mobile and immobile zone. $[s^{-1}]$

`DualPorosity_Data::porosity_immobile` = $\langle \text{abstract type: } \textcolor{red}{IT::Field:R3} \rightarrow \textcolor{red}{Real} \rangle$

Default: $\langle \text{optional} \rangle$

Porosity of the immobile zone. $[-]$

`DualPorosity_Data::init_conc_immobile` = $\langle \text{abstract type: } \textcolor{red}{IT::Field:R3} \rightarrow \textcolor{red}{Real}[n] \rangle$

Default: $\langle \text{optional} \rangle$

Initial concentration of substances in the immobile zone. $[m^{-3}kg]$

selection type: **IT::DualPorosity_Output**

Possible values:

`diffusion_rate_immobile` : Output of the field `diffusion_rate_immobile` $[s^{-1}]$ (Diffusion coefficient of non-equilibrium linear exchange between mobile and immobile zone.).

`porosity_immobile` : Output of the field `porosity_immobile` $[-]$ (Porosity of the immobile zone.).

`init_conc_immobile` : Output of the field `init_conc_immobile` $[m^{-3}kg]$ (Initial concentration of substances in the immobile zone.).

`conc_immobile` : Output of the field `conc_immobile` $[m^{-3}kg]$.

record: **IT::Semchem** implements abstract type: **IT::ReactionTerm**

Declares infos valid for all reactions. NOT SUPPORTED!!!.

Semchem::TYPE = $\langle \textit{selection: ReactionTerm_TYPE_selection} \rangle$

Default: Semchem

Sub-record selection.

Semchem::precision = $\langle \textit{Integer}[-2147483648,] \rangle$

Default: $\langle \textit{obligatory} \rangle$

How accurate should the simulation be, decimal places(?).

Semchem::temperature = $\langle \textit{Double} \rangle$

Default: $\langle \textit{obligatory} \rangle$

Isothermal reaction, thermodynamic temperature.

Semchem::temp_gf = $\langle \textit{Double} \rangle$

Default: $\langle \textit{obligatory} \rangle$

Thermodynamic parameter.

Semchem::param_afi = $\langle \textit{Double} \rangle$

Default: $\langle \textit{obligatory} \rangle$

Thermodynamic parameter.

Semchem::param_b = $\langle \textit{Double} \rangle$

Default: $\langle \textit{obligatory} \rangle$

Thermodynamic parameter.

Semchem::epsilon = $\langle \textit{Double} \rangle$

Default: $\langle \textit{obligatory} \rangle$

Thermodynamic parameter.

Semchem::time_steps = $\langle \textit{Integer}[-2147483648,] \rangle$

Default: $\langle \textit{obligatory} \rangle$

Simulation parameter.

Semchem::slow_kinetic_steps = $\langle \textit{Integer}[-2147483648,] \rangle$

Default: $\langle \textit{obligatory} \rangle$

Simulation parameter.

record: **IT::TransportOperatorSplitting_Data**

Record to set fields of the equation.

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_Data record that comes later in the boundary data array.

TransportOperatorSplitting_Data::r_set = $\langle \textit{String (generic)} \rangle$

Default: $\langle \textit{optional} \rangle$

Name of region set where to set fields.

TransportOperatorSplitting_Data::region = $\langle \textit{String (generic)} \rangle$

Default: $\langle \textit{optional} \rangle$

Label of the region where to set fields.

TransportOperatorSplitting_Data::rid = $\langle \textit{Integer}[0,] \rangle$

Default: $\langle \textit{optional} \rangle$

ID of the region where to set fields.

`TransportOperatorSplitting_Data::time` = $\langle \text{Double}[0,] \rangle$
 Default: $\langle 0.0 \rangle$
 Apply field setting in this record after this time.
 These times have to form an increasing sequence.

`TransportOperatorSplitting_Data::porosity` = $\langle \text{abstract type: } IT::Field:R3 \rightarrow Real \rangle$
 Default: $\langle optional \rangle$
 Mobile porosity $[-]$

`TransportOperatorSplitting_Data::sources_density` = $\langle \text{abstract type: } IT::Field:R3 \rightarrow Real[n] \rangle$
 Default: $\langle optional \rangle$
 Density of concentration sources. $[m^{-3}kg s^{-1}]$

`TransportOperatorSplitting_Data::sources_sigma` = $\langle \text{abstract type: } IT::Field:R3 \rightarrow Real[n] \rangle$
 Default: $\langle optional \rangle$
 Concentration flux. $[s^{-1}]$

`TransportOperatorSplitting_Data::sources_conc` = $\langle \text{abstract type: } IT::Field:R3 \rightarrow Real[n] \rangle$
 Default: $\langle optional \rangle$
 Concentration sources threshold. $[m^{-3}kg]$

`TransportOperatorSplitting_Data::bc_conc` = $\langle \text{abstract type: } IT::Field:R3 \rightarrow Real[n] \rangle$
 Default: $\langle optional \rangle$
 Boundary conditions for concentrations. $[m^{-3}kg]$

`TransportOperatorSplitting_Data::init_conc` = $\langle \text{abstract type: } IT::Field:R3 \rightarrow Real[n] \rangle$
 Default: $\langle optional \rangle$
 Initial concentrations. $[m^{-3}kg]$

`TransportOperatorSplitting_Data::transport_old_bcd_file` = $\langle \text{input file name} \rangle$
 Default: $\langle optional \rangle$
 File with mesh dependent boundary conditions (obsolete).

selection type: **IT::ConvectionTransport_Output**

Possible values:

`porosity` : Output of the field porosity $[-]$ (Mobile porosity).

`sources_density` : Output of the field sources_density $[m^{-3}kg s^{-1}]$ (Density of concentration sources.).

`sources_sigma` : Output of the field sources_sigma $[s^{-1}]$ (Concentration flux.).

`sources_conc` : Output of the field sources_conc $[m^{-3}kg]$ (Concentration sources threshold.).

`init_conc` : Output of the field init_conc $[m^{-3}kg]$ (Initial concentrations.).

`conc` : Output of the field conc $[m^{-3}kg]$.

`region_id` : Output of the field region_id $[-]$.

record: **IT::SoluteTransport_DG** implements abstract type: **IT::Transport**

DG solver for solute transport.

`SoluteTransport_DG::TYPE` = $\langle \text{selection: } \textit{Transport_TYPE_selection} \rangle$
 Default: `SoluteTransport_DG`
 Sub-record selection.

`SoluteTransport_DG::time` = $\langle \text{record: } \textit{IT::TimeGovernor} \rangle$
 Default: $\langle \textit{obligatory} \rangle$
 Time governor setting for the secondary equation.

`SoluteTransport_DG::balance` = $\langle \text{record: } \textit{IT::Balance} \rangle$
 Default: $\langle \textit{obligatory} \rangle$
 Settings for computing balance.

`SoluteTransport_DG::output_stream` = $\langle \text{record: } \textit{IT::OutputStream} \rangle$
 Default: $\langle \textit{obligatory} \rangle$
 Parameters of output stream.

`SoluteTransport_DG::substances` = $\langle \text{Array of Record: } \textit{IT::Substance} \rangle$
 Default: $\langle \textit{obligatory} \rangle$
 Names of transported substances.

`SoluteTransport_DG::solver` = $\langle \text{record: } \textit{IT::Petsc} \rangle$
 Default: $\langle \textit{obligatory} \rangle$
 Linear solver for MH problem.

`SoluteTransport_DG::input_fields` = $\langle \text{Array of Record: } \textit{IT::SoluteTransport_DG_Data} \rangle$
 Default: $\langle \textit{obligatory} \rangle$

`SoluteTransport_DG::dg_variant` = $\langle \text{selection: } \textit{IT::DG_variant} \rangle$
 Default: non-symmetric
 Variant of interior penalty discontinuous Galerkin method.

`SoluteTransport_DG::dg_order` = $\langle \textit{Integer}[0, 3] \rangle$
 Default: $\langle 1 \rangle$
 Polynomial order for finite element in DG method (order 0 is suitable if there is no diffusion/dispersion).

`SoluteTransport_DG::output_fields` = $\langle \text{Array of Selection: } \textit{IT::SoluteTransport_DG_Output} \rangle$
 Default: $\langle \textit{conc} \rangle$
 List of fields to write to output file.

record: **`IT::SoluteTransport_DG_Data`**

Record to set fields of the equation.

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 `SoluteTransport_DG_Data` record that comes later in the boundary data array.

`SoluteTransport_DG_Data::r_set` = $\langle \textit{String (generic)} \rangle$
 Default: $\langle \textit{optional} \rangle$
 Name of region set where to set fields.

`SoluteTransport_DG_Data::region` = $\langle \textit{String (generic)} \rangle$
 Default: $\langle \textit{optional} \rangle$

Label of the region where to set fields.

`SoluteTransport_DG_Data::rid` = $\langle \text{Integer}[0,] \rangle$
 Default: $\langle \text{optional} \rangle$
 ID of the region where to set fields.

`SoluteTransport_DG_Data::time` = $\langle \text{Double}[0,] \rangle$
 Default: $\langle 0.0 \rangle$
 Apply field setting in this record after this time.
 These times have to form an increasing sequence.

`SoluteTransport_DG_Data::porosity` = $\langle \text{abstract type: } IT::Field:R3 \rightarrow Real \rangle$
 Default: $\langle \text{optional} \rangle$
 Mobile porosity $[-]$

`SoluteTransport_DG_Data::sources_density` = $\langle \text{abstract type: } IT::Field:R3 \rightarrow Real[n] \rangle$
 \rangle
 Default: $\langle \text{optional} \rangle$
 Density of concentration sources. $[m^{-3}kg s^{-1}]$

`SoluteTransport_DG_Data::sources_sigma` = $\langle \text{abstract type: } IT::Field:R3 \rightarrow Real[n] \rangle$
 \rangle
 Default: $\langle \text{optional} \rangle$
 Concentration flux. $[s^{-1}]$

`SoluteTransport_DG_Data::sources_conc` = $\langle \text{abstract type: } IT::Field:R3 \rightarrow Real[n] \rangle$
 Default: $\langle \text{optional} \rangle$
 Concentration sources threshold. $[m^{-3}kg]$

`SoluteTransport_DG_Data::bc_conc` = $\langle \text{abstract type: } IT::Field:R3 \rightarrow Real[n] \rangle$
 Default: $\langle \text{optional} \rangle$
 Dirichlet boundary condition (for each substance). $[m^{-3}kg]$

`SoluteTransport_DG_Data::init_conc` = $\langle \text{abstract type: } IT::Field:R3 \rightarrow Real[n] \rangle$
 Default: $\langle \text{optional} \rangle$
 Initial concentrations. $[m^{-3}kg]$

`SoluteTransport_DG_Data::disp_l` = $\langle \text{abstract type: } IT::Field:R3 \rightarrow Real[n] \rangle$
 Default: $\langle \text{optional} \rangle$
 Longitudinal dispersivity (for each substance). $[m]$

`SoluteTransport_DG_Data::disp_t` = $\langle \text{abstract type: } IT::Field:R3 \rightarrow Real[n] \rangle$
 Default: $\langle \text{optional} \rangle$
 Transversal dispersivity (for each substance). $[m]$

`SoluteTransport_DG_Data::diff_m` = $\langle \text{abstract type: } IT::Field:R3 \rightarrow Real[n] \rangle$
 Default: $\langle \text{optional} \rangle$
 Molecular diffusivity (for each substance). $[m^2 s^{-1}]$

`SoluteTransport_DG_Data::fracture_sigma` = $\langle \text{abstract type: } IT::Field:R3 \rightarrow Real[n] \rangle$
 \rangle
 Default: $\langle \text{optional} \rangle$
 Coefficient of diffusive transfer through fractures (for each substance). $[-]$

`SoluteTransport_DG_Data::dg_penalty` = $\langle \text{abstract type: } IT::Field:R3 \rightarrow Real[n] \rangle$
 Default: $\langle \text{optional} \rangle$
 Penalty parameter influencing the discontinuity of the solution (for each substance). Its default value 1 is sufficient in most cases. Higher value diminishes the inter-element jumps. $[-]$

`SoluteTransport_DG_Data::bc_type` = $\langle \text{abstract type: } IT::Field:R3 \rightarrow Enum[n] \rangle$

Default: $\langle optional \rangle$
 Boundary condition type, possible values: inflow, dirichlet, neumann, robin.
 $[-]$
SoluteTransport_DG_Data::bc_flux = $\langle abstract\ type: IT::Field:R3 \rightarrow Real[n] \rangle$
 Default: $\langle optional \rangle$
 Flux in Neumann boundary condition. $[m^{1-d}kg s^{-1}]$
SoluteTransport_DG_Data::bc_robin_sigma = $\langle abstract\ type: IT::Field:R3 \rightarrow Real[n] \rangle$
 \rangle
 Default: $\langle optional \rangle$
 Conductivity coefficient in Robin boundary condition. $[m^{4-d}s^{-1}]$

abstract type: **IT::Field:R3** \rightarrow **Enum[n]** default descendant: **IT::FieldConstant**

Descendants:

Abstract record for all time-space functions.

IT::FieldConstant

IT::FieldFormula

IT::FieldPython

IT::FieldInterpolatedP0

IT::FieldElementwise

record: **IT::FieldConstant** implements abstract type: **IT::Field:R3** \rightarrow **Enum[n]** constructible from key: **FieldConstant::value**

R3 \rightarrow **Enum[n]** Field constant in space.

FieldConstant::TYPE = $\langle selection: Field:R3 \rightarrow Enum[n]_{TYPE_selection} \rangle$

Default: FieldConstant

Sub-record selection.

FieldConstant::value = $\langle Array [1,]\ of\ Selection: IT::TransportDG_BC_Type \rangle$

Default: $\langle obligatory \rangle$

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: **IT::TransportDG_BC_Type**

Types of boundary condition supported by the transport DG model (solute transport or heat transfer).

Possible values:

none : Homogeneous Neumann boundary condition. Zero flux

dirichlet : Dirichlet boundary condition.

neumann : Neumann boundary condition. Prescribe water outflow by the 'bc_flux' field.

robin : Robin boundary condition. Water outflow equal to $\sigma(h - h^R)$.

inflow : Prescribes the concentration in the inflow water on the inflow part of the boundary.

selection type: **IT::DG_variant**

Type of penalty term.

Possible values:

non-symmetric : non-symmetric weighted interior penalty DG method

incomplete : incomplete weighted interior penalty DG method

symmetric : symmetric weighted interior penalty DG method

selection type: **IT::SoluteTransport_DG_Output**

Output record for DG solver for solute transport.

Possible values:

porosity : Output of the field porosity $[-]$ (Mobile porosity).

sources_density : Output of the field sources_density $[m^{-3}kg s^{-1}]$ (Density of concentration sources.).

sources_sigma : Output of the field sources_sigma $[s^{-1}]$ (Concentration flux.).

sources_conc : Output of the field sources_conc $[m^{-3}kg]$ (Concentration sources threshold.).

init_conc : Output of the field init_conc $[m^{-3}kg]$ (Initial concentrations.).

disp_l : Output of the field disp_l $[m]$ (Longitudinal dispersivity (for each substance).).

disp_t : Output of the field disp_t $[m]$ (Transversal dispersivity (for each substance).).

diff_m : Output of the field diff_m $[m^2 s^{-1}]$ (Molecular diffusivity (for each substance).).

conc : Output of the field conc $[m^{-3}kg]$.

fracture_sigma : Output of the field fracture_sigma $[-]$ (Coefficient of diffusive transfer through fractures (for each substance).).

dg_penalty : Output of the field dg_penalty $[-]$ (Penalty parameter influencing the discontinuity of the solution (for each substance). Its default value 1 is sufficient in most cases. Higher value diminishes the inter-element jumps.).

region_id : Output of the field region_id $[-]$.

record: **IT::HeatTransfer_DG** implements abstract type: **IT::Transport**

DG solver for heat transfer.

HeatTransfer_DG::TYPE = $\langle selection: Transport_TYPE_selection \rangle$

Default: HeatTransfer_DG

Sub-record selection.

HeatTransfer_DG::time = $\langle record: IT::TimeGovernor \rangle$

Default: $\langle obligatory \rangle$

Time governor setting for the secondary equation.

HeatTransfer_DG::balance = $\langle record: IT::Balance \rangle$

Default: $\langle obligatory \rangle$

Settings for computing balance.

HeatTransfer_DG::output_stream = $\langle record: IT::OutputStream \rangle$

Default: $\langle obligatory \rangle$

Parameters of output stream.

HeatTransfer_DG::solver = $\langle record: IT::Petsc \rangle$

Default: $\langle obligatory \rangle$

Linear solver for MH problem.

HeatTransfer_DG::input_fields = $\langle \text{Array of Record: } \textcolor{red}{IT::HeatTransfer_DG_Data} \rangle$
 Default: $\langle \text{obligatory} \rangle$

HeatTransfer_DG::dg_variant = $\langle \text{selection: } \textcolor{red}{IT::DG_variant} \rangle$
 Default: non-symmetric
 Variant of interior penalty discontinuous Galerkin method.

HeatTransfer_DG::dg_order = $\langle \text{Integer}[0, 3] \rangle$
 Default: $\langle 1 \rangle$
 Polynomial order for finite element in DG method (order 0 is suitable if there is no diffusion/dispersion).

HeatTransfer_DG::output_fields = $\langle \text{Array of Selection: } \textcolor{red}{IT::HeatTransfer_DG_Output} \rangle$
 Default: $\langle \text{temperature} \rangle$
 List of fields to write to output file.

record: $\textcolor{red}{IT::HeatTransfer_DG_Data}$

Record to set fields of the equation.

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 HeatTransfer_DG_Data record that comes later in the boundary data array.

HeatTransfer_DG_Data::r_set = $\langle \text{String (generic)} \rangle$

Default: $\langle \text{optional} \rangle$

Name of region set where to set fields.

HeatTransfer_DG_Data::region = $\langle \text{String (generic)} \rangle$

Default: $\langle \text{optional} \rangle$

Label of the region where to set fields.

HeatTransfer_DG_Data::rid = $\langle \text{Integer}[0,] \rangle$

Default: $\langle \text{optional} \rangle$

ID of the region where to set fields.

HeatTransfer_DG_Data::time = $\langle \text{Double}[0,] \rangle$

Default: $\langle 0.0 \rangle$

Apply field setting in this record after this time.

These times have to form an increasing sequence.

HeatTransfer_DG_Data::bc_temperature = $\langle \text{abstract type: } \textcolor{red}{IT::Field:R3} \rightarrow \textcolor{red}{Real} \rangle$

Default: $\langle \text{optional} \rangle$

Boundary value of temperature. [K]

HeatTransfer_DG_Data::init_temperature = $\langle \text{abstract type: } \textcolor{red}{IT::Field:R3} \rightarrow \textcolor{red}{Real} \rangle$

Default: $\langle \text{optional} \rangle$

Initial temperature. [K]

HeatTransfer_DG_Data::porosity = $\langle \text{abstract type: } \textcolor{red}{IT::Field:R3} \rightarrow \textcolor{red}{Real} \rangle$

Default: $\langle \text{optional} \rangle$

Porosity. [–]

HeatTransfer_DG_Data::fluid_density = $\langle \text{abstract type: } \textcolor{red}{IT::Field:R3} \rightarrow \textcolor{red}{Real} \rangle$

Default: $\langle \text{optional} \rangle$

Density of fluid. [$m^{-3}kg$]

`HeatTransfer_DG_Data::fluid_heat_capacity` = $\langle \text{abstract type: } IT::Field:R3 \rightarrow Real \rangle$
 Default: $\langle optional \rangle$
 Heat capacity of fluid. $[m^2 s^{-2} K^{-1}]$

`HeatTransfer_DG_Data::fluid_heat_conductivity` = $\langle \text{abstract type: } IT::Field:R3 \rightarrow Real \rangle$
 Default: $\langle optional \rangle$
 Heat conductivity of fluid. $[m kgs^{-3} K^{-1}]$

`HeatTransfer_DG_Data::solid_density` = $\langle \text{abstract type: } IT::Field:R3 \rightarrow Real \rangle$
 Default: $\langle optional \rangle$
 Density of solid (rock). $[m^{-3} kg]$

`HeatTransfer_DG_Data::solid_heat_capacity` = $\langle \text{abstract type: } IT::Field:R3 \rightarrow Real \rangle$
 Default: $\langle optional \rangle$
 Heat capacity of solid (rock). $[m^2 s^{-2} K^{-1}]$

`HeatTransfer_DG_Data::solid_heat_conductivity` = $\langle \text{abstract type: } IT::Field:R3 \rightarrow Real \rangle$
 Default: $\langle optional \rangle$
 Heat conductivity of solid (rock). $[m kgs^{-3} K^{-1}]$

`HeatTransfer_DG_Data::disp_l` = $\langle \text{abstract type: } IT::Field:R3 \rightarrow Real \rangle$
 Default: $\langle optional \rangle$
 Longitudinal heat dispersivity in fluid. $[m]$

`HeatTransfer_DG_Data::disp_t` = $\langle \text{abstract type: } IT::Field:R3 \rightarrow Real \rangle$
 Default: $\langle optional \rangle$
 Transversal heat dispersivity in fluid. $[m]$

`HeatTransfer_DG_Data::fluid_thermal_source` = $\langle \text{abstract type: } IT::Field:R3 \rightarrow Real \rangle$
 Default: $\langle optional \rangle$
 Thermal source density in fluid. $[m^{-1} kgs^{-3}]$

`HeatTransfer_DG_Data::solid_thermal_source` = $\langle \text{abstract type: } IT::Field:R3 \rightarrow Real \rangle$
 Default: $\langle optional \rangle$
 Thermal source density in solid. $[m^{-1} kgs^{-3}]$

`HeatTransfer_DG_Data::fluid_heat_exchange_rate` = $\langle \text{abstract type: } IT::Field:R3 \rightarrow Real \rangle$
 Default: $\langle optional \rangle$
 Heat exchange rate in fluid. $[s^{-1}]$

`HeatTransfer_DG_Data::solid_heat_exchange_rate` = $\langle \text{abstract type: } IT::Field:R3 \rightarrow Real \rangle$
 Default: $\langle optional \rangle$
 Heat exchange rate of source in solid. $[s^{-1}]$

`HeatTransfer_DG_Data::fluid_ref_temperature` = $\langle \text{abstract type: } IT::Field:R3 \rightarrow Real \rangle$
 Default: $\langle optional \rangle$
 Reference temperature of source in fluid. $[K]$

`HeatTransfer_DG_Data::solid_ref_temperature` = $\langle \text{abstract type: } IT::Field:R3 \rightarrow Real \rangle$

Default: $\langle optional \rangle$
Reference temperature in solid. $[K]$

HeatTransfer_DG_Data::fracture_sigma = $\langle abstract\ type: IT::Field:R3 \rightarrow Real[n] \rangle$
Default: $\langle optional \rangle$
Coefficient of diffusive transfer through fractures (for each substance). $[-]$

HeatTransfer_DG_Data::dg_penalty = $\langle abstract\ type: IT::Field:R3 \rightarrow Real[n] \rangle$
Default: $\langle optional \rangle$
Penalty parameter influencing the discontinuity of the solution (for each substance). Its default value 1 is sufficient in most cases. Higher value diminishes the inter-element jumps. $[-]$

HeatTransfer_DG_Data::bc_type = $\langle abstract\ type: IT::Field:R3 \rightarrow Enum[n] \rangle$
Default: $\langle optional \rangle$
Boundary condition type, possible values: inflow, dirichlet, neumann, robin.
 $[-]$

HeatTransfer_DG_Data::bc_flux = $\langle abstract\ type: IT::Field:R3 \rightarrow Real[n] \rangle$
Default: $\langle optional \rangle$
Flux in Neumann boundary condition. $[m^{1-d}kg s^{-1}]$

HeatTransfer_DG_Data::bc_robin_sigma = $\langle abstract\ type: IT::Field:R3 \rightarrow Real[n] \rangle$
Default: $\langle optional \rangle$
Conductivity coefficient in Robin boundary condition. $[m^{4-d}s^{-1}]$

abstract type: **IT::Field:R3** \rightarrow **Enum[n]** default descendant: **IT::FieldConstant**

Descendants:

Abstract record for all time-space functions.

IT::FieldConstant

IT::FieldFormula

IT::FieldPython

IT::FieldInterpolatedP0

IT::FieldElementwise

selection type: **IT::HeatTransfer_DG_Output**

Selection for output fields of DG solver for heat transfer.

Possible values:

init_temperature : Output of the field init_temperature $[K]$ (Initial temperature.).

porosity : Output of the field porosity $[-]$ (Porosity.).

fluid_density : Output of the field fluid_density $[m^{-3}kg]$ (Density of fluid.).

fluid_heat_capacity : Output of the field fluid_heat_capacity $[m^2s^{-2}K^{-1}]$ (Heat capacity of fluid.).

fluid_heat_conductivity : Output of the field fluid_heat_conductivity $[mkgs^{-3}K^{-1}]$ (Heat conductivity of fluid.).

solid_density : Output of the field solid_density $[m^{-3}kg]$ (Density of solid (rock).).

solid_heat_capacity : Output of the field solid_heat_capacity $[m^2s^{-2}K^{-1}]$ (Heat capacity of solid (rock).).

solid_heat_conductivity : Output of the field solid_heat_conductivity $[mkgs^{-3}K^{-1}]$ (Heat conductivity of solid (rock).).

disp_l : Output of the field disp_l $[m]$ (Longitudal heat dispersivity in fluid.).

`disp_t` : Output of the field `disp_t` [m] (Transversal heat dispersivity in fluid.).
`fluid_thermal_source` : Output of the field `fluid_thermal_source` [$m^{-1}kg s^{-3}$] (Thermal source density in fluid.).
`solid_thermal_source` : Output of the field `solid_thermal_source` [$m^{-1}kg s^{-3}$] (Thermal source density in solid.).
`fluid_heat_exchange_rate` : Output of the field `fluid_heat_exchange_rate` [s^{-1}] (Heat exchange rate in fluid.).
`solid_heat_exchange_rate` : Output of the field `solid_heat_exchange_rate` [s^{-1}] (Heat exchange rate of source in solid.).
`fluid_ref_temperature` : Output of the field `fluid_ref_temperature` [K] (Reference temperature of source in fluid.).
`solid_ref_temperature` : Output of the field `solid_ref_temperature` [K] (Reference temperature in solid.).
`temperature` : Output of the field `temperature` [K].
`fracture_sigma` : Output of the field `fracture_sigma` $[-]$ (Coefficient of diffusive transfer through fractures (for each substance).).
`dg_penalty` : Output of the field `dg_penalty` $[-]$ (Penalty parameter influencing the discontinuity of the solution (for each substance). Its default value 1 is sufficient in most cases. Higher value diminishes the inter-element jumps.).
`region_id` : Output of the field `region_id` $[-]$.

0.1 Simple md support

showcase of **strong** and *em* fonts (or *both*), links to [Google](#)
Simple lists:

- hi
- hello
- greetings

Also numbered:

1. foo
2. bar
3. stuff

also code support:

```
x = 0
x = 2 + 2
what is x
```

Additionally link to Records, AbstractRecords and Selections. You can also **reference** their fields (for example record key)

link to **Root (Record)** and its key: **problem (Record key)** looks like this
 or like this:

- `pause_after_run` (Record key)
- `problem` (Record key)
- `SequentialCoupling` (Record)
- `PartTool` (Selection)
- `diff_m` (Record key)

Using latex in md:

bold and *italic* font

or like this: $x = \frac{1+y}{1+2z^2}$ bigger?

$$x = \frac{1+y}{1+2z^2}$$

or

$$\frac{1}{1 + \frac{1}{2 + \frac{1}{3+x}}} + \frac{1}{1 + \frac{1}{2 + \frac{1}{3+x}}}$$

or

$$e^x \approx 1 + x + x^2/2! + \\ + x^3/3! + x^4/4! + \\ + x^5/5!$$

ca asc