LA-UR-06-7048

Title: *Quick Reference Guide: PFLOTRAN 1.0 (LA-CC 06-093) Multiphase-Multicomponent-Multiscale Massively Parallel Reactive Transport Code*

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DRAFT

1 Introduction

2 PFLOTRAN Keywords

The PFLOTRAN input file construction is based on keywords. Lines beginning with a colon (:) are treated as comments. Each entry to the input file must begin in the first column. Keywords `SKIP` and `NOSKIP` are used to skip over sections of the input file. Blank lines may occur in input file. Alternate keyword spelling is indicated in round brackets ( ). Input options are indicated in square brackets [ ], as well as default values. Curly brackets { } indicate the result of invoking the corresponding keyword. Always refer to source code when in doubt!

Initial and boundary conditions and material properties are assigned to spatial regions using a novel *coupler* approach. In this approach, initial and boundary conditions (keyword CONDITION) are assigned to regions (keyword REGION) using keywords INITIAL_CONDITION and BOUNDARY_CONDITION. Material properties (keyword MATERIAL) are assigned to regions using the keyword STRATIGRAPHY.

Keyword	Status	Comments
BOUNDARY_CONDITION		
BREAKTHROUGH		
BRINE (BRIN)		
CHECKPOINT		
COMPUTE_STATISTICS (STATISTICS)		
CONDITION		
DATASET		
DEBUG		
DIFF		
DTST		
DXYZ		
GRAVITY		
GRID		
HDF5		
IMOD		
INVERT_Z (INVERTZ)		
INITIAL_CONDITION		
LINEAR_SOLVER		

Keyword: BOUNDARY_CONDITION

BOUNDARY_CONDITION

REGION region_name

CONDITION condition_name

TYPE [initial, boundary, source_sink]

FACE [WEST, EAST, NORTH, SOUTH, BOTTOM, TOP]

END

Keyword: BREAKTHROUGH (BRK)

BREAKTHROUGH

REGION region_name

VELOCITY {print_velocities == PETSC_TRUE}

(., /, END)

Keyword: BRINE (BRIN)

BRIN, BRINE m_nacl [MOLAL, MASS, MOLE]

Keyword: CHECKPOINT

CHECKPOINT checkpoint_frequency

Keyword: COMPUTE_STATISTICS (STATISTICS)

COMPUTE_STATISTICS, STATISTICS {compute_statistics = .true.}

Keyword: CONDITION (COND)

CONDITION (COND) condition_name

UNITS

s, sec, min, hr, d, day, y, yr

mm, cm, m, met, meter, dm, km

Pa, KPa

m/s, m/yr

C, K

M, mol/L

KJ/mol

(., /, END)

CLASS [flow, transport (tran)]

CYCLIC {is_cyclic = .true.}

INTERPOLATION step linear

TYPE

PRESSURE (PRES, PRESS) [dirichlet, neumann, mass, hydrostatic (hydro, hydrostat), static, zero_gradient, seepage]

FLUX [dirichlet, neumann, mass, hydrostatic (hydro, hydrostat), static, zero_gradient, seepage]

TEMPERATURE (TEMP) [dirichlet, neumann, mass, hydrostatic (hydro, hydrostat), static, zero_gradient, seepage]

CONCENTRATION (CONC) [dirichlet, neumann, mass, hydrostatic (hydro, hydrostat), static, zero_gradient, seepage]

ENTHALPY (H) [dirichlet, neumann, mass, hydrostatic (hydro, hydrostat), static, zero_gradient, seepage]

(., /, END)

TIME

IPHASE

DATUM (DATM)

[Continued]

Keyword: CONDITION (COND) [Continued]

GRADIENT (GRAD)

PRESSURE (PRES, PRESS)

FLUX

TEMPERATURE (TEMP)

CONCENTRATION (CONC)

ENTHALPY (H)

(., /, END)

TEMPERATURE (TEMP)

ENTHALPY (H)

PRESSURE (PRES, PRESS)

FLUX (VELOCITY, VEL)

CONCENTRATION (CONC)

(., /, END)

Keyword: DATASET

DATASET [permx, permy, permz] [permx_filename, permy_filename, permz_filename]

Keyword: DEBUG

DEBUG

PRINT_SOLUTION (VECVIEW_SOLUTION, VIEW_SOLUTION)

PRINT_RESIDUAL (VECVIEW_RESIDUAL,VIEW_RESIDUAL)

PRINT_JACOBIAN (MATVIEW_JACOBIAN, VIEW_JACOBIAN)

PRINT_JACOBIAN_NORM (NORM_JACOBIAN)

PRINT_COUPLERS (PRINT_COUPLER)

PRINT_JACOBIAN_DETAILED (MATVIEW_JACOBIAN_DETAILED, VIEW_JACOBIAN_DETAILED)

PRINT_NUMERICAL_DERIVATIVES (VIEW_NUMERICAL_DERIVATIVES)

END

Keyword: DIFF

DIFF difaq delhaq

Keyword: DTST

DTST dt_min

dt1, dt2, dt3, . . . , dt_max

Keyword: DXYZ

DXYZ [STRUCTURED_GRID, AMR_GRID]

dx0

dy0

dz0

Keyword: GRAVITY (GRAV)

GRAVITY (GRAV) gravity

Keyword: GRID

GRID

TYPE [structured, unstructured, amr]

NXYZ nx ny nz

FILE

END

Keyword: HDF5

HDF5 [VELO, FLUX]

Keyword: IMOD

IMOD mod

Keyword: INVERT_Z (INVERTZ)

INVERT_Z (INVERTZ) {invert_z_axis = .true.}

Keyword: INITIAL_CONDITION

INITIAL_CONDITION

REGION region_name

CONDITION condition_name

TYPE [initial, boundary, source_sink]

FACE [WEST, EAST, NORTH, SOUTH, BOTTOM, TOP]

END

Keyword: LINEAR_SOLVER

LINEAR_SOLVER

TRAN, TRANSPORT (tran_solver) / DEFAULT (flow_solver)

SOLVER_TYPE (SOLVER, KRYLOV_TYPE, KRYLOV, KSP, KSP_TYPE)

NONE (PREONLY)

GMRES

BCGS (BICGSTAB, BI-CGSTAB)

PRECONDITIONER_TYPE (PRECONDITIONER, PC, PC_TYPE)

ILU (PCILU)

LU (PCLU)

BJACOBI (BLOCK_JACOBI)

ASM (ADDITIVE_SCHWARTZ)

PCASM

ATOL

RTOL

DTOL

MAXIT

(., /, END)

Keyword: MATERIAL (MATERIALS, PHIK)

MATERIAL (MATERIALS, PHIK)

name id icap ithrm por tor permx permy permz permpwr

(., /, END)

Keyword: MODE

MODE [RICHARDS_LITE, RICHARDS, MPH]

Keyword: NEWTON_SOLVER

NEWTON_SOLVER

TRAN, TRANSPORT (tran_solver) / DEFAULT (flow_solver)

INEXACT_NEWTON

NO_PRINT_CONVERGENCE

NO_INF_NORM (NO_INFINITY_NORM)

NO_FORCE_ITERATION

PRINT_DETAILED_CONVERGENCE

ATOL

RTOL

STOL

DTOL

ITOL (INF_TOL, ITOL_RES, INF_TOL_RES)

ITOL_UPDATE (INF_TOL_UPDATE)

MAXIT

MAXF

(., /, END)

Keyword: NUMERICAL_JACOBIAN

NUMERICAL_JACOBIAN {numerical_derivatives = .true.}

Keyword: ORIGIN (ORIG)

ORIGIN (ORIG) X_DIRECTION Y_DIRECTION Z_DIRECTION

Keyword: OVERWRITE_RESTART_TRANSPORT

OVERWRITE_RESTART_TRANSPORT {overwrite_restart_transport = .true.}

Keyword: REGION

REGION region_name

BLOCK i1 i2 j1 j2 k1 k2

COORDINATE x-coordinate y-coordinate z-coordinate

FILE filename

LIST (not implemented)

FACE [WEST, EAST, NORTH, SOUTH, BOTTOM, TOP]

END

Keyword: RESTART

RESTART restart_file restart_time

Keyword: RICH

RICH pref

Keyword: SATURATION_FUNCTION (SATURATION_FUNCTIONS, PCKR)

SATURATION_FUNCTION (SATURATION_FUNCTIONS, PCKR)

id icaptype [(Sr[np],np=1,nphase), Sr] pckrm alpha pcwmax pbetac pwrprm

(., /, END)

Keyword: SOURCE_SINK

SOURCE_SINK

REGION region_name

CONDITION condition_name

TYPE [initial, boundary, source_sink]

FACE [WEST, EAST, NORTH, SOUTH, BOTTOM, TOP]

END

Keyword: STRATIGRAPHY (STRATA)

STRATIGRAPHY (STRATA)

REGION region_name

MATERIAL material_name

INACTIVE

(., /, END)

Keyword: TECP

TECP [VELO, FLUX]

Keyword: THRM (THERMAL_PROPERTY, THERMAL_PROPERTIES)

THRM (THERMAL_PROPERTY, THERMAL_PROPERTIES)

id rock_density spec_heat therm_cond_dry therm_cond_wet tort_bin_diff vap_air_diff_coef exp_binary_diff

(., /, END)

Keyword: TIME

TIME	[s, m, h, d, mo, y] [every #]
	t1, t2, t3, ...

Keyword: TIMESTEPPER

TIMESTEPPER

NUM_STEPS_AFTER_TS_CUT [5]

MAX_STEPS [999999]

TS_ACCELERATION [5]

MAX_TS_CUTS [16]

MAX_PRESSURE_CHANGE [5.d4]

MAX_TEMPERATURE_CHANGE [5.d0]

MAX_CONCENTRATION_CHANGE [1.d0]

MAX_SATURATION_CHANGE [0.5d0]

(., /, END)

Keyword: TRAN

TRAN	ntrandof

Keyword: UNIFORM_VELOCITY

UNIFORM_VELOCITY vlx vly vlz

Keyword: USE_TOUCH_OPTIONS

USE_TOUCH_OPTIONS {use_touch_options = .true.}

Keyword: WALLCLOCK_STOP

WALLCLOCK_STOP wallclock_stop_time

Example Input File

```
:Description: 2D problem for saturated layered medium
:
:MODE RICHARDS
MODE RICHARDS_LITE
TRAN 1
:
:NUMERICAL_JACOBIAN
:INEXACT_NEWTON
:USE_TOUCH_OPTIONS
:
:CHECKPOINT 1000
:RESTART steady.chk 0.d0
:OVERWRITE_RESTART_TRANSPORT
:COMPUTE_STATISTICS
:USE_TOUCH_OPTIONS
:WALLCLOCK_STOP 0.d0
:
DEBUG
:MATVIEW_JACOBIAN
:VECVIEW_RESIDUAL
:VECVIEW_SOLUTION
:PRINT_COUPLERS
END
:
GRID
TYPE structured
NXYZ 450 1 4430
END
```

```
:
ORIGIN 0.d0 0.d0 0.d0
:
NEWTON_SOLVER
RTOL 1.d-5
ATOL 1.d-7
STOL 1.d-10
:ITOL_RES 1.d-8
:ITOL_UPDATE 0.05d0  ! Pa
NO_INFINITY_NORM
:NO_FORCE_ITERATION
:NO_PRINT_CONVERGENCE
:PRINT_DETAILED_CONVERGENCE
MAXIT 20
END
:noskip
:
NEWTON_SOLVER TRANSPORT
:RTOL 1.d-50
ATOL 1.d-50
STOL 1.d-50
ITOL_RES 1.d-8
:ITOL_UPDATE 5.d0  ! Pa
:NO_INFINITY_NORM
:NO_FORCE_ITERATION
:NO_PRINT_CONVERGENCE
:PRINT_DETAILED_CONVERGENCE
MAXIT 10
END
:
TIMESTEPPER
TS_ACCELERATION 8
END
:
:HDF5 !VELO !FLUX
TECP VELO !FLUX
:
DXYZ
0.02d0
1.d0
0.002d0
:
:  d0[m^2/s] delhaq[kJ/mol]
```

```
DIFF  1.D-9       12.6
:
: Richards Equation Pref
RICH 101325.
:
SATURATION_FUNCTIONS
: van Genuchten
:id itype swir   m      alpha     pcwmax betac pwr
 1  1     0.1600 0.3391 7.2727d-4 1.e8   0.d0  1.d0
 2  1     0.1299 0.7479 1.4319d-4 1.e8   0.d0  1.d0
: Brooks-Corey
:id itype swir   lambda alpha     pcwmax betac pwr
: 1  2     0.1600 1.97   7.2727d-4 1.e8   0.d0  1.d0
: 2  2     0.1299 0.5193 1.4319d-4 1.e8   0.d0  1.d0
END

THERMAL_PROPERTIES
:ithm rho    cpr     ckdry cksat tau cdiff   cexp
  1   2.76e3 1000.e0 0.5   0.5   0.5 2.13d-5 1.8
END
:
MATERIALS
:name id icap ithm por  tau permx  permy  permz  permpwr
tuff 1  1    1    0.2 0.5 1.d-19 1.d-19 1.d-19 1.d0
END
:
:
:TIME y every 10.
TIME y
0.1 0.25 0.5 0.75 1.
:
DTST 1.d-8
1. 0.001d0
:
:define regions-----------------------------------------------------------------
:
REGION all
BLOCK 1 450 1 1 1 4430
END

REGION Left
FACE west
BLOCK 1 1 1 1 3931 4430
```

```
END

REGION Right
FACE east
BLOCK 450 450 1 1 1 500
END

:define initial and boundary conditions-------------------------------------

:flow-----------------------

CONDITION initial
CLASS flow
TYPE
PRESSURE hydrostatic
END
DATUM 0.d0 0.d0 10.d0
PRESSURE 101325.d0
END

CONDITION Left
CLASS flow
TYPE
PRESSURE neumann
END
PRESSURE 1.5854896d-7 ! 5000 mm/yr
END

CONDITION Right
CLASS flow
TYPE
PRESSURE neumann
END
PRESSURE -1.5854896d-7 ! 5000 mm/yr
END

:transport-----------------

CONDITION initial_c
CLASS transport
CONCENTRATION 1.d-8
END
```

```
CONDITION outlet_c
CLASS transport
TYPE
CONCENTRATION zero_gradient
END
CONCENTRATION 1.d-8
END

CONDITION inlet_c
CLASS transport
CONCENTRATION 1.d0
END

:set initial and boundary conditions----------------------------------------

:flow-----------------------

: initial condition
INITIAL_CONDITION
CONDITION initial
REGION all
END

BOUNDARY_CONDITION
CONDITION Left
REGION Left
END

BOUNDARY_CONDITION
CONDITION initial
REGION Right
END

:transport------------------

: initial condition
INITIAL_CONDITION
CONDITION initial_c
REGION all
END

BOUNDARY_CONDITION
CONDITION inlet_c
```

```
REGION Left
END

BOUNDARY_CONDITION
CONDITION outlet_c
REGION Right
END

:set material properties-------------------------------------------------

STRATA
MATERIAL tuff
REGION all
END

:read in permeability field----------------------------------------------

DATASET permx perm_inv.dat
DATASET permy perm_inv.dat
DATASET permz perm_inv.dat
```