

LA-UR-06-7048

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|-------------------|---|
| <i>Title:</i> | <i>Quick Reference Guide: PFLOTRAN 1.0 (LA-CC 06-093)</i> <i>Multiphase-Multicomponent-Multiscale Massively Parallel</i> <i>Reactive Transport Code</i> |
| <i>Author(s):</i> | SciDAC-2 Project (PI: Peter C. Lichtner, lichtner@lanl.gov) |
| <i>Contacts:</i> | Glenn Hammond (glenn.hammond@pnnl.gov) Richard Mills (rmills@ornl.gov) |
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DRAFT

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1 Introduction

PFLOTRAN solves a system of generally nonlinear partial differential equations describing multiphase, multicomponent and multiscale reactive flow and transport in porous materials. The code is designed to run on massively parallel computing architectures as well as workstations and laptops. Parallelization is achieved through domain decomposition using the PETSc (Portable Extensible Toolkit for Scientific Computation) libraries for the parallelization framework (Balay et al., 1997).

2 Installation

The following instructions should aid in installing openmpi, PETSc, HDF5 and PFLOTRAN on a UNIX or Mac computer running MacOSX 10.4 or later.

2.1 Openmpi

Set environment variables PKGS and MPI_HOME and the appropriate PATH:

```
setenv PKGS /Users/lichtner/petsc/packages
setenv MPI_HOME $PKGS/openmpi/openmpi-1.2.5-gcc-4.0.1-absoft-10.1
setenv PATH \"$PKGS/openmpi/openmpi-1.2.5-gcc-4.0.1-absoft-10.1:$PATH
setenv F90 f90
setenv F77 'f90 -YEXT_NAMES=LCS -YEXT_SFX= -f'
setenv FC 'f90 -YEXT_NAMES=LCS -YEXT_SFX= -f'
setenv CC gcc
```

Configure using:

```
./configure --prefix=$PKGS/openmpi/openmpi-1.2.6-gcc-4.0.1-absoft-10.1
```

Finally, compile, check installation and install:

```
make
make check
make install
```

2.2 PETSc

PFLOTRAN uses the Developer version of PETSc. To install PETSc first set the environment variables PETSC_DIR and PETSC_ARCH:

```
setenv PETSC_DIR /Users/lichtner/petsc/petsc-dev
setenv PETSC_ARCH Intel_MacOSX10.5
```

Configure PETSc on a Mac using openmpi and Fortran 90 Absoft 10.1:

```
./config/configure.py
--with-blas-lapack-lib="-framework vecLib"
--with-mpi-dir=$PKGS/openmpi/openmpi-1.2.6-gcc-4.0.1-absoft-10.1
--with-debugging=0
--with-shared=0
```

Compile and test the PETSc installation with:

```
make all test
```

Optionally install PETSc:

```
make install
```

2.3 HDF5

To install HDF5 set the following environment variables:

```
setenv HDF5_INCLUDE $PKGS/hdf/hdf5-1.6.7-gcc-4.0.1-absoft-10.1/include
setenv HDF5_LIB $PKGS/hdf/hdf5-1.6.7-gcc-4.0.1-absoft-10.1/lib
setenv CC $MPI_HOME/bin/mpicc
setenv F9X $MPI_HOME/bin/mpif90
setenv CFLAGS -fno-strict-aliasing
setenv FFLAGS ""
```

```
./configure --enable-fortran
--prefix=$PKGS/hdf/hdf5-1.6.7-gcc-4.0.1-absoft-10.1
--disable-debug --enable-production --enable-parallel
--enable-static --disable-shared
```

```
make
make check
make install
```

2.4 PFLOTTRAN

Compile PFLOTTRAN using the command

```
make [hdf5=1] pflotran
```

Create input file `pflotran.in` and run PFLOTTRAN with the command:

```
mpirun -n #proc pflotran
```

where `#proc` is the desired number of processor cores.

3 Creating the Input File: PFLOTTRAN Keywords

The PFLOTTRAN 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 | Description |
|---------------------------------|-------------|
| 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
MATERIAL (MATERIALS, PHIK)
MODE
NEWTON_SOLVER
NUMERICAL_JACOBIAN
ORIG, ORIGIN
OVERWRITE_RESTART_TRANSPORT
REGION
RESTART
RICH
SATURATION_FUNCTION (SATURATION_FUNCTION, PCKR)
SOURCE_SINK
STRATIGRAPHY (STRATA)
TECP
THRM, THERMAL_PROPERTY (THERMAL_PROPERTIES)
TIME
TIMESTEPER
TRAN
UNIFORM_VELOCITY
USE_TOUCH_OPTIONS
WALLCLOCK_STOP

3.1 Keyword: BOUNDARY_CONDITION

BOUNDARY_CONDITION

REGION region_name

FLOW_CONDITION condition_name

TRANSPORT_CONDITION condition_name

TYPE [initial, boundary, source_sink]

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

END

3.2 Keyword: BREAKTHROUGH (BRK)

BREAKTHROUGH

REGION region_name

VELOCITY {print_velocities == PETSC_TRUE}

(., /, END)

3.3 Keyword: BRINE (BRIN)

BRIN, BRINE m_nacl [MOLAL, MASS, MOLE]

3.4 Keyword: CHECKPOINT

CHECKPOINT checkpoint_frequency

3.5 Keyword: COMPUTE_STATISTICS (STATISTICS)

COMPUTE_STATISTICS, STATISTICS {compute_statistics = .true.}

3.6 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]

3.7 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)

3.8 Keyword: DATASET

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

3.9 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

3.10 Keyword: DIFF

DIFF difaq delhaq

3.11 Keyword: DTST

DTST Δt_{\min}

$t_1 \Delta t_1$

$t_2 \Delta t_2$

...

$t_N \Delta t_{\max}$

3.12 Keyword: DXYZ

| | |
|-------------|-----------------------------|
| DXYZ | [STRUCTURED_GRID, AMR_GRID] |
| | dx0 |
| | dy0 |
| | dz0 |

3.13 Keyword: GRAVITY (GRAV)

| | |
|-----------------------|---------|
| GRAVITY (GRAV) | gravity |
|-----------------------|---------|

3.14 Keyword: GRID

| |
|--------------------------------------|
| GRID |
| TYPE [structured, unstructured, amr] |
| NXYZ nx ny nz |
| FILE |
| END |

3.15 Keyword: HDF5

| | |
|-------------|--------------|
| HDF5 | [VELO, FLUX] |
|-------------|--------------|

3.16 Keyword: IMOD

| | |
|-------------|-----|
| IMOD | mod |
|-------------|-----|

3.17 Keyword: INVERT_Z (INVERTZ)

```
INVERT_Z (INVERTZ) {invert_z_axis = .true.}
```

3.18 Keyword: INITIAL_CONDITION

```
INITIAL_CONDITION
```

```
    REGION region_name
```

```
    FLOW_CONDITION condition_name
```

```
    TRANSPORT_CONDITION condition_name
```

```
    TYPE [initial, boundary, source_sink]
```

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

```
END
```

3.19 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)

3.20 Keyword: MATERIAL (MATERIALS, PHIK)

MATERIAL (MATERIALS, PHIK)

name id icap ithrm por tor permx permy permz permpwr

(., /, END)

3.21 Keyword: MODE

MODE [RICHARDS_LITE, RICHARDS, MPH]

3.22 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)

3.23 Keyword: NUMERICAL_JACOBIAN

NUMERICAL_JACOBIAN {numerical_derivatives = .true.}

3.24 Keyword: ORIGIN (ORIG)

ORIGIN (ORIG) X_DIRECTION Y_DIRECTION Z_DIRECTION

3.25 Keyword: OVERWRITE_RESTART_TRANSPORT

```
OVERWRITE_RESTART_TRANSPORT {overwrite_restart_transport = .true.}
```

3.26 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
```

3.27 Keyword: RESTART

```
RESTART      restart_file restart_time
```

3.28 Keyword: RICH

```
RICH         pref
```

3.29 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)
```

3.30 Keyword: SOURCE_SINK

SOURCE_SINK

REGION region_name

CONDITION condition_name

TYPE [initial, boundary, source_sink]

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

END

3.31 Keyword: STRATIGRAPHY (STRATA)

STRATIGRAPHY (STRATA)

REGION region_name

MATERIAL material_name

INACTIVE

(., /, END)

3.32 Keyword: TECP

TECP [VELO, FLUX]

3.33 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)

3.34 Keyword: TIME

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

3.35 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) |

3.36 Keyword: TRAN

| | |
|-------------|----------|
| TRAN | ntrandof |
|-------------|----------|

3.37 Keyword: UNIFORM_VELOCITY

| | |
|-------------------------|-------------|
| UNIFORM_VELOCITY | vlx vly vlz |
|-------------------------|-------------|

3.38 Keyword: USE_TOUCH_OPTIONS

```
USE_TOUCH_OPTIONS {use_touch_options = .true.}
```

3.39 Keyword: WALLCLOCK_STOP

```
WALLCLOCK_STOP wallclock_stop_time
```

Example Input File

```
:Description: 3D toy problem for richards equation
:
MODE RICHARDS_LITE
TRAN 1
:
CHECKPOINT 1000
RESTART steady_68_125_20_Scope3.chk 0.d0
OVERWRITE_RESTART_TRANSPORT
OVERWRITE_RESTART_FLOW_PARAMS
WALLCLOCK_STOP 3.95
:
GRID
TYPE structured
NXYZ 68 125 20
END
:
ORIGIN 0.d0 0.d0 90.d0
:
NEWTON_SOLVER FLOW
:RTOL 1.d-50
RTOL 1.d-5
:ATOL 1.d-50
ATOL 1.d-8
:STOL 1.d-50
STOL 1.d-6
:ITOL_RES 1.d-4
:ITOL_UPDATE 0.5d0 ! Pa
NO_INFINITY_NORM
```

```
NO_FORCE_ITERATION
:NO_PRINT_CONVERGENCE
:PRINT_DETAILED_CONVERGENCE
MAXIT 20
END
:
NEWTON_SOLVER TRANSPORT
:RTOL 1.d-50
RTOL 1.d-6
:ATOL 1.d-50
:STOL 1.d-50
:STOL 1.d-6
:ITOL_RES 1.d-8
NO_INFINITY_NORM
:NO_FORCE_ITERATION
:NO_PRINT_CONVERGENCE
:PRINT_DETAILED_CONVERGENCE
MAXIT 10
END
:
LINEAR_SOLVER FLOW
:KSP_TYPE gmres
:RTOL 1.d-50
:ATOL 1.d-10
END
:
TIMESTEPER
TS_ACCELERATION 8
END
:
:HDF5 !VELO !FLUX
TECP VELO !FLUX
:
DXYZ
19.8529411765d0
20.d0
1.d0
:
: 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
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
: Hanford 1 1 1 0.20 0.5 7.387d-9 7.387d-9 7.387d-10 1.d0
Hanford 1 1 1 0.20 0.5 7.387d-10 7.387d-10 7.387d-10 1.d0
Unit2 2 2 1 0.25 0.5 0.d0 0.d0 0.d0 1.d0
Unit3 3 2 1 0.25 0.5 0.d0 0.d0 0.d0 1.d0
Unit4 4 2 1 0.25 0.5 0.d0 0.d0 0.d0 1.d0
Unit5 5 2 1 0.25 0.5 4.221d-11 4.221d-11 4.221d-12 1.d0
Unit6 6 2 1 0.25 0.5 1.052d-14 1.052d-14 1.052d-15 1.e0
Unit7 7 2 1 0.25 0.5 4.523d-11 4.523d-11 4.523d-12 1.e0
Unit8 8 2 1 0.25 0.5 5.259d-17 5.259d-17 5.259d-18 1.e0
Unit9 9 2 1 0.25 0.5 5.259d-17 5.259d-17 5.259d-18 1.e0
Unit10 10 2 1 0.25 0.5 1.d-20 1.d-20 1.d-20 1.e0
END

:
: TIME h
: 100000.
TIME h every 168
7500.

:
: DTST 1.d-6
: 1. 100000.
DTST 1.d-2
1. 1.d0

:
REGION all
BLOCK 1 68 1 125 1 20
END

REGION West

```

```
FILE input_68_125_20_Scope3.h5  
END
```

```
REGION East  
FILE input_68_125_20_Scope3.h5  
END
```

```
REGION North  
FILE input_68_125_20_Scope3.h5  
END
```

```
REGION South  
FILE input_68_125_20_Scope3.h5  
END
```

```
REGION Top  
FILE input_68_125_20_Scope3.h5  
END
```

```
REGION North_Pond_West_Trench  
FILE input_68_125_20_Scope3.h5  
END
```

```
REGION North_Pond_East_Trench  
FILE input_68_125_20_Scope3.h5  
END
```

```
:REGION Plume  
:FILE input_68_125_20_Scope3.h5  
:END
```

```
REGION Plume_Source  
FILE input_68_125_20_Scope3.h5  
:BLOCK 60 62 70 72 15 17  
END
```

```
REGION 399-1-1  
COORDINATE 1208.69 1784.40 100.0  
END
```

```
REGION 399-1-2  
COORDINATE 876.57 1599.94 100.0  
END
```


REGION 399-2-1
COORDINATE 1199.61 1304.67 100.0
END

REGION 399-2-2
COORDINATE 1159.62 1480.95 100.0
END

REGION 399-3-9
COORDINATE 1186.58 1098.39 100.0
END

REGION 399-3-12
COORDINATE 911.44 1196.74 100.0
END

REGION 399-4-1
COORDINATE 870.96 784.91 100.0
END

REGION 399-4-7
COORDINATE 1179.54 661.80 100.0
END

REGION 399-4-9
COORDINATE 1176.30 919.13 100.0
END

REGION 399-5-1
COORDINATE 360.22 899.80 100.0
END

REGION ifc
COORDINATE 979.57 1302.39 100.0
END

BREAKTHROUGH
REGION 399-1-1
END

BREAKTHROUGH
REGION 399-1-2

END

BREAKTHROUGH
REGION 399-2-1
END

BREAKTHROUGH
REGION 399-2-2
END

BREAKTHROUGH
REGION 399-3-9
END

BREAKTHROUGH
REGION 399-3-12
END

BREAKTHROUGH
REGION 399-4-1
END

BREAKTHROUGH
REGION 399-4-9
END

BREAKTHROUGH
REGION 399-5-1
END

BREAKTHROUGH
REGION ifc
VELOCITY
END

CONDITION initial
UNITS Pa,C,M,yr
CLASS flow
TYPE
PRESSURE hydrostatic
TEMPERATURE dirichlet
CONCENTRATION dirichlet
END

```
:DATUM file initial_data.datum
DATUM 1.2294770e+003 9.4611630e+002 1.0559964e+002
GRADIENT
:PRESSURE file initial_data.gradient
PRESSURE 1.9538819e-004 2.8407287e-004 0.0000000e+000
END
PRESSURE 101325.d0
TEMPERATURE 25.d0
CONCENTRATION 1.d-6
END

CONDITION river
CLASS flow
TYPE
PRESSURE seepage
TEMPERATURE dirichlet
CONCENTRATION dirichlet
END
INTERPOLATION linear
DATUM file river.datum
:DATUM 1.2294770e+003 9.4611630e+002 1.0559964e+002
GRADIENT
PRESSURE file river.gradient_adj
:PRESSURE 0.d0 0.00027389 0.d0
END
PRESSURE 101325.d0
TEMPERATURE 25.d0
CONCENTRATION 1.d-6
END

CONDITION west
CLASS flow
TYPE
PRESSURE hydrostatic
TEMPERATURE dirichlet
CONCENTRATION dirichlet
END
INTERPOLATION linear
DATUM file well_data.datum
:DATUM 2.1149088e+002 1.2272915e+003 1.0548061e+002
GRADIENT
PRESSURE file well_data.gradient
:PRESSURE -7.8414067e-004 3.4105428e-004 0.0000000e+000
```

END

PRESSURE 101325.d0

TEMPERATURE 25.d0

CONCENTRATION 1.d-6

END

CONDITION north

CLASS flow

TYPE

PRESSURE hydrostatic

TEMPERATURE dirichlet

CONCENTRATION dirichlet

END

INTERPOLATION linear

DATUM file north.datum

:DATUM 0. 2500. 106.0805113

GRADIENT

PRESSURE file north.gradient

:PRESSURE -4.09472e-05 0. 0.

END

PRESSURE 101325.d0

TEMPERATURE 25.d0

CONCENTRATION 1.d-6

END

CONDITION south

CLASS flow

TYPE

PRESSURE hydrostatic

TEMPERATURE dirichlet

CONCENTRATION dirichlet

END

INTERPOLATION linear

DATUM file south.datum

:DATUM 0 0 105.2278756

GRADIENT

PRESSURE file south.gradient

:PRESSURE 8.34319e-05 0. 0.

END

PRESSURE 101325.d0

TEMPERATURE 25.d0

CONCENTRATION 1.d-6

END

```
CONDITION recharge
CLASS flow
TYPE
PRESSURE neumann
TEMPERATURE dirichlet
CONCENTRATION dirichlet
END
FLUX file recharge.txt
:FLUX 1.756d-9
TEMPERATURE 25.d0
CONCENTRATION 1.d-6
END
```

```
CONDITION plume
CLASS flow
TYPE
PRESSURE neumann
END
FLUX 0.d0
END
```

```
CONDITION north_pond_west_trench
CLASS flow
TYPE
PRESSURE neumann
TEMPERATURE dirichlet
CONCENTRATION dirichlet
END
FLUX file north_pond_west_trench.txt
:FLUX 4.500d-5
TEMPERATURE 25.d0
CONCENTRATION 1.d-6
END
```

```
CONDITION north_pond_east_trench
CLASS flow
TYPE
PRESSURE neumann
TEMPERATURE dirichlet
CONCENTRATION dirichlet
END
FLUX file north_pond_east_trench.txt
```

```
:FLUX 0.d0  
TEMPERATURE 25.d0  
CONCENTRATION 1.d-6  
END
```

```
CONDITION river_c  
CLASS transport  
CONCENTRATION 1.d-40  
END
```

```
CONDITION west_c  
CLASS transport  
CONCENTRATION 1.d-40  
END
```

```
CONDITION initial_c  
CLASS transport  
CONCENTRATION 1.d-40  
END
```

```
CONDITION plume_c  
CLASS transport  
CONCENTRATION 1.d0  
END
```

```
: initial condition  
INITIAL_CONDITION  
FLOW_CONDITION initial  
TRANSPORT_CONDITION initial_c  
REGION all  
END
```

```
: inland boundary condition  
BOUNDARY_CONDITION  
FLOW_CONDITION west  
TRANSPORT_CONDITION initial_c  
REGION West  
END
```

```
: river boundary condition  
BOUNDARY_CONDITION  
FLOW_CONDITION river  
TRANSPORT_CONDITION initial_c
```

REGION East
END

: north boundary condition
BOUNDARY_CONDITION
FLOW_CONDITION north
TRANSPORT_CONDITION initial_c
REGION North
END

: south boundary condition
BOUNDARY_CONDITION
FLOW_CONDITION south
TRANSPORT_CONDITION initial_c
REGION South
END

: recharge boundary condition
BOUNDARY_CONDITION
FLOW_CONDITION recharge
TRANSPORT_CONDITION initial_c
REGION Top
END

: north pond west trench boundary condition
BOUNDARY_CONDITION
FLOW_CONDITION north_pond_west_trench
TRANSPORT_CONDITION initial_c
REGION North_Pond_West_Trench
END

: north pond east trench boundary condition
BOUNDARY_CONDITION
FLOW_CONDITION north_pond_east_trench
TRANSPORT_CONDITION initial_c
REGION North_Pond_East_Trench
END

: plume source
SOURCE_SINK
FLOW_CONDITION plume
TRANSPORT_CONDITION plume_c
REGION Plume_Source

END

STRATA

MATERIAL input_68_125_20_Scope3.h5

END

:read in permeability field-----

DATASET permx perm_inv.dat

DATASET permy perm_inv.dat

DATASET permz perm_inv.dat

4 PFLOTTRAN Objects

This section gives an overview in alphabetical order of the objects and their data structures used in PFLOTTRAN. The upper most object is **Simulation** followed by **Realization**, followed by **Level**, **Patch** and **Grid**.

| Object | Description |
|--------------------------------|-------------|
| Breakthrough | |
| Condition | |
| Connection | |
| Coupler | |
| Discretization | |
| Field | |
| Grid | |
| Level | |
| Logging | |
| Material | |
| Option | |
| Patch | |
| Realization | |
| Region | |
| Richards | |
| Richards_lite | |

[Simulation](#)
[Solver](#)
[Stepper](#)
[Strata](#)
[Structured_grid](#)
[Waypoint](#)

4.1 Breakthrough

```

type, public :: breakthrough_type
  ! all added variables must be included in BreakthroughCreateFromBreakthrough
  PetscInt :: id
  PetscTruth :: print_velocities
  character(len=MAXWORDLENGTH) :: name
  character(len=MAXWORDLENGTH) :: region_name
  type(region_type), pointer :: region
  type(breakthrough_type), pointer :: next
end type breakthrough_type

type, public :: breakthrough_list_type
  PetscInt :: num_breakthroughs
  type(breakthrough_type), pointer :: first
  type(breakthrough_type), pointer :: last
  type(breakthrough_type), pointer :: array(:)
end type breakthrough_list_type

```

4.2 Condition

```

type, public :: condition_dataset_type
  PetscInt :: rank
  logical :: is_transient
  logical :: is_cyclic
  PetscInt :: interpolation_method
  PetscReal, pointer :: times(:)
  PetscReal, pointer :: values(:, :)
  PetscReal, pointer :: cur_value(:)
  PetscInt :: cur_time_index
  PetscInt :: max_time_index

```

```

end type condition_dataset_type

type, public :: condition_type
  PetscInt :: id ! id from which condition can be referenced
  character(len=MAXWORDLENGTH) :: class ! character string describing class of
                                         condition
  PetscInt :: iclass ! integer id for class
  logical :: sync_time_with_update
  character(len=MAXWORDLENGTH) :: name ! name of condition (e.g. initial,
                                         recharge)

  PetscInt :: num_sub_conditions
  PetscInt :: iphase
  PetscInt, pointer :: itype(:)
  character(len=MAXWORDLENGTH) :: time_units
  character(len=MAXWORDLENGTH) :: length_units
  type(sub_condition_type), pointer :: pressure
  type(sub_condition_type), pointer :: temperature
  type(sub_condition_type), pointer :: concentration
  type(sub_condition_type), pointer :: enthalpy
  type(sub_condition_ptr_type), pointer :: sub_condition_ptr(:)
  type(condition_type), pointer :: next ! pointer to next condition_type for
                                         linked-lists
end type condition_type

type, public :: sub_condition_type
  PetscInt :: itype ! integer describing type of condition
  character(len=MAXWORDLENGTH) :: ctype ! character string describing type of
                                         condition
  character(len=MAXWORDLENGTH) :: units ! units

  type(condition_dataset_type) :: datum
  type(condition_dataset_type) :: gradient
  type(condition_dataset_type) :: dataset

end type sub_condition_type

type, public :: sub_condition_ptr_type
  type(sub_condition_type), pointer :: ptr
end type sub_condition_ptr_type

type, public :: condition_ptr_type
  type(condition_type), pointer :: ptr
end type condition_ptr_type

```

```

type, public :: condition_list_type
  PetscInt :: num_conditions
  type(condition_type), pointer :: first
  type(condition_type), pointer :: last
  type(condition_ptr_type), pointer :: array(:)
end type condition_list_type

```

4.3 Connection

```

type, public :: connection_set_type
  PetscInt :: id
  PetscInt :: itype                ! connection type (boundary, internal,
                                   source sink

  PetscInt :: num_connections
  PetscInt, pointer :: id_up(:)    ! list of ids of upwind cells
  PetscInt, pointer :: id_dn(:)    ! list of ids of downwind cells
  PetscReal, pointer :: dist(:, :) ! list of distance vectors,
                                   size(-1:3,num_connections) where
                                   !   -1 = fraction upwind
                                   !   0 = magnitude of distance
                                   !   1-3 = components of unit vector

  PetscReal, pointer :: area(:)    ! list of areas of faces normal to
                                   distance vectors

!   PetscReal, pointer :: velocity(:, :) ! velocity scalars for each phase
  type(connection_set_type), pointer :: next
end type connection_set_type

```

! pointer data structure required for making an array of region pointers in F90

```

type, public :: connection_set_ptr_type
  type(connection_set_type), pointer :: ptr                ! pointer to the
                                                            connection_set_type

end type connection_set_ptr_type

```

```

type, public :: connection_set_list_type
  PetscInt :: num_connection_objects
  type(connection_set_type), pointer :: first
  type(connection_set_type), pointer :: last
  type(connection_set_ptr_type), pointer :: array(:)
end type connection_set_list_type

```

4.4 Coupler

```

type, public :: coupler_type
  PetscInt :: id                      ! id of coupler
  PetscInt :: itype                   ! integer defining type
  character(len=MAXWORDLENGTH) :: ctype ! character string defining type
  character(len=MAXWORDLENGTH) :: condition_name ! character string
                                              defining name of condition to be applied
  character(len=MAXWORDLENGTH) :: region_name ! character string
                                              defining name of region to be applied
  PetscInt :: icondition              ! id of condition in condition array/list
  PetscInt :: iregion                 ! id of region in region array/list
  PetscInt :: iface                   ! for structured grids only
  PetscInt, pointer :: aux_int_var(:, :) ! auxilliary array for integer value
  PetscReal, pointer :: aux_real_var(:, :) ! auxilliary array for real values
  type(condition_type), pointer :: condition ! pointer to condition in
                                              condition array/list
  type(region_type), pointer :: region ! pointer to region in
                                      region array/list
  type(connection_type), pointer :: connection ! pointer to an array/list
                                              of connections
  type(coupler_type), pointer :: next ! pointer to next coupler
end type coupler_type

type, public :: coupler_ptr_type
  type(coupler_type), pointer :: ptr
end type coupler_ptr_type

type, public :: coupler_list_type
  PetscInt :: num_couplers
  type(coupler_type), pointer :: first
  type(coupler_type), pointer :: last
  type(coupler_ptr_type), pointer :: array(:)
end type coupler_list_type

```

4.5 Discretization

```

type, public :: discretization_type
  PetscInt :: itype ! type of discretization (e.g. structured, unstructured,
                  etc.)
  character(len=MAXWORDLENGTH) :: ctype
  type(grid_type), pointer :: grid ! pointer to a grid object

```

```

    type(amrgrid_type), pointer :: amrgrid ! pointer to an amr grid object
    DM :: dm_1_dof, dm_nflowdof, dm_ntrandof
end type discretization_type

```

4.6 Field

```

type, public :: field_type

!geh material id
! 1 degree of freedom
Vec :: porosity0, porosity_loc
Vec :: tor_loc
Vec :: ithrm_loc
Vec :: icap_loc
Vec :: iphas_loc, iphas_old_loc

Vec :: perm_xx_loc, perm_yy_loc, perm_zz_loc
Vec :: perm0_xx, perm0_yy, perm0_zz, perm_pow

Vec :: saturation_loc, density_loc

Vec :: volume

! residual vectors
Vec :: flow_r
Vec :: tran_r

! Solution vectors
Vec :: flow_xx, flow_xx_loc, flow_dxx, flow_yy, flow_accum
Vec :: tran_xx, tran_xx_loc, tran_dxx, tran_yy, tran_accum

end type field_type

```

4.7 Grid

```

type, public :: grid_type

character(len=MAXWORDLENGTH) :: ctype
PetscInt :: itype ! type of grid (e.g. structured, unstructured, etc.)

```

```

PetscInt :: nmax    ! Total number of nodes in global domain
PetscInt :: nlmax   ! Total number of non-ghosted nodes in local domain.
PetscInt :: ngmax   ! Number of ghosted & non-ghosted nodes in local domain.

!nL2G : not collective, local processor: local => ghosted local
!nG2L : not collective, local processor: ghosted local => local
!nG2N : collective, ghosted local => global index , used for
!
!               matsetvaluesblocked ( not matsetvaluesblockedlocal)
!nL2A : collective, local => natural index, used for initialization
!
!               and source/sink setup
PetscInt, pointer :: nL2G(:), nG2L(:), nL2A(:)
PetscInt, pointer :: nG2A(:)

PetscReal, pointer :: x(:), y(:), z(:)

PetscReal :: x_min, x_max, y_min, y_max, z_min, z_max

PetscInt, pointer :: hash(:, :, :)
PetscInt :: num_hash_bins

type(structured_grid_type), pointer :: structured_grid
type(unstructured_grid_type), pointer :: unstructured_grid

type(connection_list_type), pointer :: internal_connection_list

end type grid_type

```

4.8 Level

```

type, public :: level_type

    PetscInt :: id
    type(patch_list_type), pointer :: patch_list
    type(level_type), pointer :: next

end type level_type

! pointer data structure required for making an array of level pointers in F90
type, public :: level_ptr_type
    type(level_type), pointer :: ptr           ! pointer to the level_type
end type level_ptr_type

```

```
type, public :: level_list_type
  PetscInt :: num_level_objects
  type(level_type), pointer :: first
  type(level_type), pointer :: last
  type(level_ptr_type), pointer :: array(:)
end type level_list_type
```

4.9 Logging

```
type, public :: logging_type

  PetscInt :: stage(10)

  PetscInt :: class_pflotran

  PetscEvent :: event_init
  PetscEvent :: event_setup

  PetscEvent :: event_restart
  PetscEvent :: event_checkpoint

  PetscEvent :: event_condition_read
  PetscEvent :: event_condition_read_values

  PetscEvent :: event_h5dread_f
  PetscEvent :: event_h5dwrite_f
  PetscEvent :: event_read_indices_hdf5
  PetscEvent :: event_map_indices_hdf5
  PetscEvent :: event_hash_create
  PetscEvent :: event_hash_map
  PetscEvent :: event_read_real_array_hdf5
  PetscEvent :: event_read_int_array_hdf5
  PetscEvent :: event_write_real_array_hdf5
  PetscEvent :: event_write_int_array_hdf5
  PetscEvent :: event_read_array_hdf5
  PetscEvent :: event_write_struct_dataset_hdf5
  PetscEvent :: event_region_read_hdf5
  PetscEvent :: event_region_read_ascii
  PetscEvent :: event_material_read_hdf5

  PetscEvent :: event_output_tecplot
  PetscEvent :: event_output_hdf5
```

```

    PetscEvent :: event_output_str_grid_tecplot
    PetscEvent :: event_output_write_tecplot
    PetscEvent :: event_output_write_flux_tecplot
    PetscEvent :: event_output_get_var_from_array
    PetscEvent :: event_output_get_cell_vel
    PetscEvent :: event_output_vec_tecplot
    PetscEvent :: event_output_breakthrough
    PetscEvent :: event_output_coordinates_hdf5

end type logging_type

```

4.10 Material

```

type, public :: material_type
    PetscInt :: id
    character(len=MAXWORDLENGTH) :: name
    PetscReal :: permeability(3,3)
    PetscReal :: permeability_pwr
    PetscReal :: porosity
    PetscReal :: tortuosity
    PetscInt :: ithrm
    PetscInt :: icap
    type(material_type), pointer :: next
end type material_type

```

```

type, public :: material_ptr_type
    type(material_type), pointer :: ptr
end type material_ptr_type

```

```

type, public :: thermal_property_type
    PetscInt :: id
    PetscReal :: rock_density
    PetscReal :: spec_heat
    PetscReal :: therm_cond_dry
    PetscReal :: therm_cond_wet
    PetscReal :: pore_compress
    PetscReal :: pore_expansivity
    PetscReal :: tort_bin_diff
    PetscReal :: vap_air_diff_coef
    PetscReal :: exp_binary_diff
    PetscReal :: enh_binary_diff_coef
    type(thermal_property_type), pointer :: next

```



```

end type thermal_property_type

type, public :: saturation_function_type
  PetscInt :: id
  character(len=MAXWORDLENGTH) :: saturation_function_ctype
  PetscInt :: saturation_function_itype
  character(len=MAXWORDLENGTH) :: permeability_function_ctype
  PetscInt :: permeability_function_itype
  PetscReal, pointer :: Sr(:)
  PetscReal :: m
  PetscReal :: lambda
  PetscReal :: alpha
  PetscReal :: pcwmax
  PetscReal :: betac
  PetscReal :: power
  PetscInt :: ihist
  PetscReal :: BC_pressure_low
  PetscReal :: BC_pressure_high
  PetscReal :: BC_spline_coefficients(4)
  type(saturation_function_type), pointer :: next
end type saturation_function_type

type, public :: saturation_function_ptr_type
  type(saturation_function_type), pointer :: ptr
end type saturation_function_ptr_type

```

4.11 Option

```

type, public :: option_type

  PetscMPIInt :: myrank                ! rank in PETSC_COMM_WORLD
  PetscMPIInt :: commsize              ! size of PETSC_COMM_WORLD

  ! defines the mode (e.g. mph, richards, vadose, etc.
  character(len=MAXWORDLENGTH) :: flowmode
  PetscInt :: iflowmode
  character(len=MAXWORDLENGTH) :: tranmode
  PetscInt :: itranmode

  PetscInt :: nphase
  PetscInt :: nflowdof
  PetscInt :: nspec

```

```

PetscInt :: nrandof
PetscInt :: ncomp

PetscReal :: uniform_velocity(3)

! Program options
PetscTruth :: use_matrix_free ! If true, do not form the Jacobian.

PetscInt :: imod

PetscTruth :: use_isoth

character(len=MAXWORDLENGTH) :: generalized_grid
logical :: use_generalized_grid

PetscReal :: flow_time, tran_time, time ! The time elapsed in the simulation.
PetscReal :: flow_dt, tran_dt, dt ! The size of the time step.

! PetscReal, pointer :: tplot(:)
PetscReal, pointer :: tfac(:)
! An array of multiplicative factors that specify how to increase time step.

PetscInt :: iblkfmt ! blocked format

! Basically our target number of newton iterations per time step.
PetscReal :: dpmxe, dtmpmxe, dsmxe, dcmxe !maximum allowed changes in field vars.
PetscReal :: dpmax, dtmpmax, dsmax, dcmax

PetscReal :: scale
PetscReal, pointer :: rock_density(:), cpr(:), dencpr(:), ckdry(:), ckwet(:), &
    tau(:), cdiff(:), cexp(:)
PetscReal, pointer :: swir(:), lambda(:), alpha(:), pckrm(:), pcwmax(:), &
    pcbetac(:), pwrprm(:), sir(:, :)
PetscInt, pointer :: icaptype(:)

PetscReal :: m_nacl
PetscReal :: difaq, delhaq, gravity(3), fmwh2o= 18.0153D0, fmwa=28.96D0, &
    fmwco2=44.0098D0, eqkair, ret=1.d0, fc=1.d0

PetscInt :: ideriv
PetscReal :: tref, pref

```

```
PetscReal :: disp

!  table lookup
PetscInt :: itable=0

PetscTruth :: restart_flag
PetscReal :: restart_time
character(len=MAXWORDLENGTH) :: restart_file
PetscTruth :: checkpoint_flag
PetscInt :: checkpoint_frequency

PetscLogDouble :: start_time
PetscTruth :: wallclock_stop_flag
PetscLogDouble :: wallclock_stop_time

PetscInt :: log_stage(10)

logical :: numerical_derivatives
logical :: compute_statistics
logical :: use_touch_options
logical :: overwrite_restart_transport
PetscInt :: io_handshake_buffer_size

character(len=MAXWORDLENGTH) :: permx_filename
character(len=MAXWORDLENGTH) :: permy_filename
character(len=MAXWORDLENGTH) :: permz_filename

end type option_type

type, public :: output_option_type

character(len=2) :: tunit
PetscReal :: tconv

logical :: print_hdf5
logical :: print_hdf5_velocities
logical :: print_hdf5_flux_velocities

logical :: print_tecplot
logical :: print_tecplot_velocities
logical :: print_tecplot_flux_velocities

PetscInt :: plot_number
```

```

    character(len=MAXWORDLENGTH) :: plot_name

end type output_option_type

```

4.12 Patch

```

type, public :: patch_type

    PetscInt :: id

    ! thiese arrays will be used by all modes, mode-specific arrays should
    ! go in the auxilliary data stucture for that mode
    PetscInt, pointer :: imat(:)
    PetscReal, pointer :: internal_velocities(:, :)
    PetscReal, pointer :: boundary_velocities(:, :)

    type(grid_type), pointer :: grid

    type(region_list_type), pointer :: regions

    type(coupler_list_type), pointer :: transport_boundary_conditions
    type(coupler_list_type), pointer :: transport_initial_conditions
    type(coupler_list_type), pointer :: transport_source_sinks

    type(coupler_list_type), pointer :: flow_boundary_conditions
    type(coupler_list_type), pointer :: flow_initial_conditions
    type(coupler_list_type), pointer :: flow_source_sinks

    type(strata_list_type), pointer :: strata
    type(breakthrough_list_type), pointer :: breakthrough

    type(auxilliary_type) :: aux

    type(patch_type), pointer :: next

end type patch_type

! pointer data structure required for making an array of patch pointers in F90
type, public :: patch_ptr_type
    type(patch_type), pointer :: ptr          ! pointer to the patch_type
end type patch_ptr_type

```

```
type, public :: patch_list_type
  PetscInt :: num_patch_objects
  type(patch_type), pointer :: first
  type(patch_type), pointer :: last
  type(patch_ptr_type), pointer :: array(:)
end type patch_list_type
```

4.13 Realization

```
type, public :: realization_type

  type(discretization_type), pointer :: discretization
  type(level_list_type), pointer :: level_list
  type(patch_type), pointer :: patch

  type(option_type), pointer :: option
  type(field_type), pointer :: field
  type(pflow_debug_type), pointer :: debug
  type(output_option_type), pointer :: output_option

  type(region_list_type), pointer :: regions
  type(condition_list_type), pointer :: flow_conditions
  type(condition_list_type), pointer :: transport_conditions

  type(material_type), pointer :: materials
  type(material_ptr_type), pointer :: material_array(:)
  type(thermal_property_type), pointer :: thermal_properties
  type(saturation_function_type), pointer :: saturation_functions
  type(saturation_function_ptr_type), pointer :: saturation_function_array(:)

  type(waypoint_list_type), pointer :: waypoints

end type realization_type
```

4.14 Region

```
type, public :: block_type
  PetscInt :: i1,i2,j1,j2,k1,k2
  type(block_type), pointer :: next
end type block_type
```

```

type, public :: region_type
  PetscInt :: id
  character(len=MAXWORDLENGTH) :: name
  character(len=MAXWORDLENGTH) :: filename
  PetscInt :: i1,i2,j1,j2,k1,k2
  PetscReal :: coordinate(3)
  PetscInt :: iface
  PetscInt :: num_cells
  PetscInt, pointer :: cell_ids(:)
  PetscInt, pointer :: faces(:)
  type(region_type), pointer :: next
end type region_type

```

```

type, public :: region_ptr_type
  type(region_type), pointer :: ptr
end type region_ptr_type

```

```

type, public :: region_list_type
  PetscInt :: num_regions
  type(region_type), pointer :: first
  type(region_type), pointer :: last
  type(region_type), pointer :: array(:)
end type region_list_type

```

4.15 Richards

```

type, public :: richards_auxvar_type
  PetscReal :: pres
  PetscReal :: temp
  PetscReal :: sat
  PetscReal :: den
  PetscReal :: den_kg
  PetscReal :: avgmw
  PetscReal :: h
  PetscReal :: u
  PetscReal :: pc
!   PetscReal :: vis
!   PetscReal :: dvis_dp
!   PetscReal :: kr
!   PetscReal :: dkr_dp
  PetscReal :: kvr

```

```

    PetscReal :: dsat_dp
    PetscReal :: dden_dp
    PetscReal :: dden_dt
    PetscReal :: dkvr_dp
    PetscReal :: dkvr_dt
    PetscReal :: dh_dp
    PetscReal :: dh_dt
    PetscReal :: du_dp
    PetscReal :: du_dt
    PetscReal, pointer :: xmol(:)
    PetscReal, pointer :: diff(:)
end type richards_auxvar_type

type, public :: richards_type
    PetscInt :: n_zero_rows
    PetscInt, pointer :: zero_rows_local(:), zero_rows_local_ghosted(:)

    logical :: aux_vars_up_to_date
    logical :: inactive_cells_exist
    PetscInt :: num_aux, num_aux_bc
    type(richards_auxvar_type), pointer :: aux_vars(:)
    type(richards_auxvar_type), pointer :: aux_vars_bc(:)
end type richards_type

```

4.16 Richards_lite

```

type, public :: richards_lite_auxvar_type
    PetscReal :: pres
    PetscReal :: temp
    PetscReal :: sat
    PetscReal :: den
    PetscReal :: den_kg
    PetscReal :: avgmw
    PetscReal :: pc
!    PetscReal :: vis
!    PetscReal :: dvis_dp
!    PetscReal :: kr
!    PetscReal :: dkr_dp
    PetscReal :: kvr
    PetscReal :: dsat_dp
    PetscReal :: dden_dp
    PetscReal :: dkvr_dp

```

```

end type richards_lite_auxvar_type

type, public :: richards_lite_type
  PetscInt :: n_zero_rows
  PetscInt, pointer :: zero_rows_local(:), zero_rows_local_ghosted(:)

  logical :: aux_vars_up_to_date
  logical :: inactive_cells_exist
  PetscInt :: num_aux, num_aux_bc
  type(richards_lite_auxvar_type), pointer :: aux_vars(:)
  type(richards_lite_auxvar_type), pointer :: aux_vars_bc(:)
end type richards_lite_type

```

4.17 Simulation

```

type, public :: simulation_type

  type(realization_type), pointer :: realization
  type(stepper_type), pointer :: flow_stepper
  type(stepper_type), pointer :: tran_stepper

end type simulation_type

```

4.18 Solver

```

type, public :: solver_type
  PetscReal :: linear_atol      ! absolute tolerance
  PetscReal :: linear_rtol      ! relative tolerance
  PetscReal :: linear_dtol      ! divergence tolerance
  PetscInt  :: linear_maxit     ! maximum number of iterations

  PetscReal :: newton_atol      ! absolute tolerance
  PetscReal :: newton_rtol      ! relative tolerance
  PetscReal :: newton_stol      ! relative tolerance (relative to previous
                                ! iteration)
  PetscReal :: newton_dtol      ! divergence tolerance
  PetscReal :: newton_inf_res_tol ! infinity tolerance for residual
  PetscReal :: newton_inf_upd_tol ! infinity tolerance for update
  PetscInt  :: newton_maxit     ! maximum number of iterations
  PetscInt  :: newton_maxf      ! maximum number of function evaluations

```



```

        ! Jacobian matrix
Mat :: J
MatFDColoring :: matfdcoloring
        ! Coloring used for computing the Jacobian via finite differences.

! PETSc nonlinear solver context
SNES :: snes
KSPTType :: ksp_type
PCType :: pc_type
KSP :: ksp
PC :: pc

PetscTruth :: inexact_newton

PetscTruth :: print_convergence
PetscTruth :: print_detailed_convergence
PetscTruth :: check_infinity_norm
PetscTruth :: force_at_least_1_iteration

end type solver_type

```

4.19 Stepper

```

type, public :: stepper_type

PetscInt :: steps      ! The number of time-steps taken by the code.
PetscInt :: nstepmax   ! Maximum number of timesteps taken by the code.
PetscInt :: icut_max   ! Maximum number of timestep cuts within one time step.
PetscInt :: ndtcmx     ! Steps needed after cutting to increase time step
PetscInt :: newtcum    ! Total number of Newton steps taken.
PetscInt :: icutcum    ! Total number of cuts in the timestep taken.
PetscInt :: iaccel     ! Accelerator index

PetscReal :: dt_min
PetscReal :: dt_max

type(solver_type), pointer :: solver

type(waypoint_type), pointer :: cur_waypoint

type(convergence_context_type), pointer :: convergence_context

```

```
end type stepper_type
```

4.20 Strata

```
type, public :: strata_type
  PetscInt :: id                ! id of strata
  logical :: active
  character(len=MAXWORDLENGTH) :: material_name ! character string defining
                                                name of material to be applied
  character(len=MAXWORDLENGTH) :: region_name   ! character string defining
                                                name of region to be applied
  PetscInt :: imaterial          ! id of material in material array/list
  PetscInt :: iregion            ! id of region in region array/list
  type(material_type), pointer :: material      ! pointer to material in
                                                material array/list
  type(region_type), pointer :: region          ! pointer to region in region
                                                array/list
  type(strata_type), pointer :: next            ! pointer to next strata
end type strata_type

type, public :: strata_ptr_type
  type(strata_type), pointer :: ptr
end type strata_ptr_type

type, public :: strata_list_type
  PetscInt :: num_strata
  type(strata_type), pointer :: first
  type(strata_type), pointer :: last
  type(strata_ptr_type), pointer :: array(:)
end type strata_list_type
```

4.21 Structured_grid

```
type, public :: structured_grid_type

  PetscInt :: nx, ny, nz      ! Global domain dimensions of the grid.
  PetscInt :: nxy, nmax      ! nx * ny, nx * ny * nz
  PetscInt :: npx, npy, npz ! Processor partition in each direction.
  PetscInt :: nlx, nly, nlz ! Local grid dimension w/o ghost nodes.
```

```

PetscInt :: ngx, ngy, ngz ! Local grid dimension with ghost nodes.
PetscInt :: nxs, nys, nzs
    ! Global indices of non-ghosted corner (starting) of local domain.
PetscInt :: ngxs, ngys, ngzs
    ! Global indices of ghosted starting corner of local domain.
PetscInt :: nxe, nye, nze, ngxe, ngye, ngze
    ! Global indices of non-ghosted/ghosted ending corner of local domain.
PetscInt :: nlxy, nlxz, nlyz
PetscInt :: ngxxy, ngxz, ngxyz

PetscInt :: istart, jstart, kstart, iend, jend, kend
    ! istart gives the local x-index of the non-ghosted starting (lower left)
    ! corner. iend gives the local x-index of the non-ghosted ending
    ! corner. jstart, jend correspond to y-index, kstart, kend to z-index.

PetscInt :: nlmax ! Total number of non-ghosted nodes in local domain.
PetscInt :: ngmax ! Number of ghosted & non-ghosted nodes in local domain.

PetscReal :: origin(3)

PetscReal, pointer :: dx0(:), dy0(:), dz0(:)

logical :: invert_z_axis

PetscReal, pointer :: dx(:), dy(:), dz(:), dxg(:), dyg(:), dzg(:) ! Grid spacings

PetscFortranAddr p_samr_patch ! pointer to a SAMRAI patch object

end type structured_grid_type

```

4.22 Waypoint

```

type, public :: waypoint_type
    PetscReal :: time
    logical :: print_output
    type(output_option_type), pointer :: output_option
    logical :: update_bcs
    logical :: update_srcs
    PetscReal :: dt_max
    logical :: final ! any waypoint after this will be deleted
    type(waypoint_type), pointer :: prev
    type(waypoint_type), pointer :: next

```

```
end type waypoint_type

type, public :: waypoint_list_type
  PetscInt :: num_waypoints
  type(waypoint_type), pointer :: first
  type(waypoint_type), pointer :: last
  type(waypoint_type), pointer :: array(:)
end type waypoint_list_type
```

5 FAQ

5.1 *iobuf* load errors

It may be the case that the ‘iobuf’ module is causing problems. That is a module that, if it’s loaded, links with an IO buffering library. It can speed up IO considerably, but there have been some bugs (hopefully fixed) identified with it before. It is loaded by default. You might want to try a ‘module unload’ of that before building PFLOTRAN, and seeing if that works. Unfortunately, it may be necessary to mess with the configuration files for the PETSc builds to make sure that you don’t link with the iobuf library.

6 References

Balay S, Eijkhout V, Gropp WD, McInnes LC and Smith BF (1997) Modern Software Tools in Scientific Computing, Eds. Arge E, Bruaset AM and Langtangen HP (Birkhäuser Press), pp. 163–202.