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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>
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1 Introduction

PFLOTTRAN 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 PFLOTTRAN 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-4.3.0-absoft-10.1
setenv PATH \ $PKGS/openmpi/openmpi-1.2.5-gcc-4.3.0-absoft-10.1:\$PATH
setenv F90 f90
setenv CC gcc
```

Configure using:

```
./configure --prefix=$PKGS/openmpi/openmpi-1.2.5-gcc-4.3.0-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-1.2.5-gcc-4.3.0-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-4.3.0-absoft-10.1/include
setenv HDF5_LIB $PKGS/hdf/hdf5-1.6.7-gcc-4.3.0-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-4.3.0-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
TIMESTEP
TRAN
UNIFORM_VELOCITY
USE_TOUCH_OPTIONS
WALLCLOCK_STOP

3.1 Keyword: BOUNDARY_CONDITION

BOUNDARY_CONDITION

REGION region_name

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
```

```
    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  icaltype [(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: 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
```

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 :: ntrandof
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 :: ndtcum     ! 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, ngx, ngy, ngze
    ! Global indices of non-ghosted/ghosted ending corner of local domain.
PetscInt :: nlxy, nlxz, nlyz
PetscInt :: ngxz, ngxz, ngyz

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.