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

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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 labtops. 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

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 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-1.2.5-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 enviroment variables `PETSC_DIR` and `PETSC_ARCH`:

```
setenv PETSC_DIR /Users/lichtner/petsc/petsc-dev

setenv PETSC_ARCH Intel_MacOSX10.4.11
```

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 PESTc 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 PFLOTRAN

Compile PFLOTRAN using the command

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

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

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

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

3 Creating the Input File: 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	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
TIMESTEPPER
TRAN
UNIFORM_VELOCITY
USE_TOUCH_OPTIONS
WALLCLOCK_STOP

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
```

4 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 (Birkhaüser Press), pp. 163–202.

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 are 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.