Coupled hydrogeophysical modelling using PFLOTRAN-E4D

Michael Tso

Lancaster University and British Geological Survey

May 3, 2018

Lancaster Environment Centre | Lancaster University

British Geological Survey
NATURAL ENVIRONMENT RESEARCH COUNCIL

About me

- 3rd year PhD student at Lancaster University (Andrew Binley, Oliver Kuras (BGS))
- **PhD project:** Enhancing the information content of geophysical data in nulcear site characterisation
- Nuclear Decommissioning Authority (NDA) PhD bursary

Acknowledgement

- Tim Johnson (Pacific Northwest National Laboratory, USA)
- Xingyuan Chen (Pacific Northwest National Laboratory, USA)
- Xuehang Song (Pacific Northwest National Laboratory, USA)

Overview of presentation

- **Goal:** Introduce the basic concepts and implementation of coupled hydrogeophysical modelling, using PFLOTRAN-E4D as an example
- Why coupled hydrogeophysical modelling?
- A flow and transport code: PFLOTRAN
- A geophysical (i.e. ERT) code: E4D
- Coupling
- A worked example
- Discussion

Why coupled hydrogeophysical modelling?

- Forward modelling
- Geophysical methods provides better coverage and resolution than tradtional point-based methods
- But geophysical properties is often not our ultimate quantity of interest (QoI)
- Coupled modelling allows one to get the geophysical response given the subsurface condition
- Data assimilation

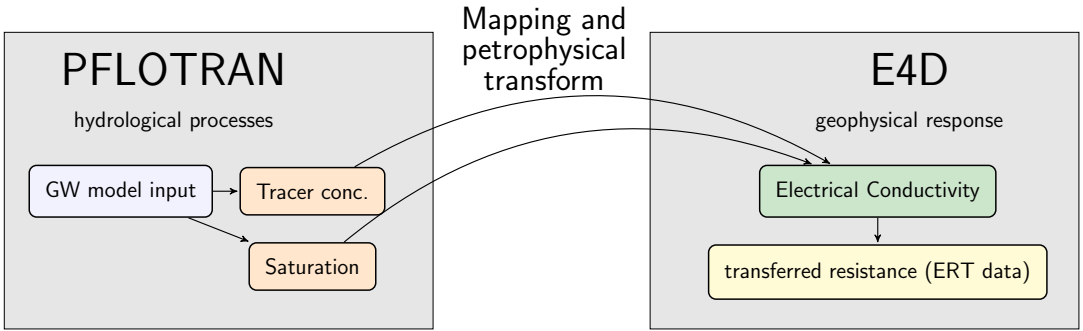
- FLOw and TRANsport
- PETSc — highly scalable
- General multi-phase code, long history of application at Hanford and other US government sites
- runs on Linux-like machines only
- A forward model... no built-in inversion or DA capabilities
- Data visualization: HDF5 (use VisIt or packages) and Tecplot point (i.e. ASCII)

E4D

- parallel ERT code
- inversion modules included (many options)
- allows inclusion of metallic structure
- runs on Linux-like machines, but also via **cygwin**
- Data visualization: Exodus II (use VisIt or Paraview)

Hydrogeophysical coupling

Workflow



PFLOTRAN-E4D coupling I

The theory (governing equations)

- Single-phase variably saturated flow is based on the Richards equation with the form

$$\frac{\partial}{\partial t}(\varphi s \rho) + \boldsymbol{\nabla} \cdot (\rho \boldsymbol{q}) = 0$$

- The Darcy velocity $\boldsymbol{q}$ is given by

$$\boldsymbol{q} = -\frac{k k_r}{\mu} \boldsymbol{\nabla}(p - \rho g z)$$

- Conservative solute transport in the liquid phase is based on the advection-dispersion equation

$$\frac{\partial}{\partial t}(\varphi s C) + \boldsymbol{\nabla} \cdot (\boldsymbol{q} - \varphi s \boldsymbol{D} \boldsymbol{\nabla}) C = 0$$

PFLOTRAN-E4D coupling II

The theory (governing equations)

- The direct-current electrical potential arising from a given current source is given by the Poisson equation

$$\nabla \cdot \sigma_b(\boldsymbol{r}) \nabla \varphi(\boldsymbol{r}) \; = \; -\nabla \cdot J(r)$$

- Petrophysical transform using Archie's Law:

$$\sigma_b \; = \; \frac{1}{a} \Phi^m S_w^n \sigma_w$$

PFLOTRAN-E4D coupling

The theory (mapping and interpolation)

- Set up an interpolation matrix
- At specified times, map fluid conductivity from PFLOTRAN to E4D
- Tri-linear interpolation of the values of fluid conductivity at each of the eight PFLOTRAN cell centres (rectangular grid)

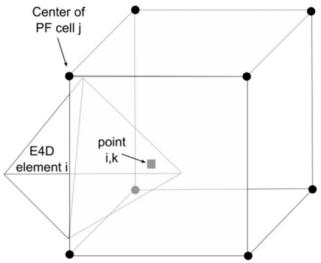


Fig. 5. Components used to interpolate bulk conductivity from the PFLOTRAN mesh to the E4D mesh.

PFLOTRAN-E4D coupling[1]

Option 1: PFLOTRAN built-in

- **What does it do?** At specified times, interpolate tracer concentration and saturation from PFLOTRAN to the E4D mesh, convert to EC, and run E4D forward model.
- Included in current PFLOTRAN release
- Just replace SUBSURFACE by HYDROGEOPHYCIS in the PFLOTRAN input card

[1] Johnson T.C. et al. (2017) PFLOTRAN-E4D: A parallel open source PFLOTRAN module for simulating time-lapse electrical resistivity data, *Computers & Geosciences*

PFLOTRAN-E4D coupling

Option 1: PFLOTRAN built-in (inputs and outputs)

- Needs all PFLOTRAN and E4D input files, plus
  - list of times to run E4D (list_files.txt)
  - E4D elementwise Archie's parameters (archies.txt)
  - PFLOTRAN node locations (pf_mesh.txt)
- Outputs
  - survey files (e4d__XXXX.0000000000.dpd), where XXXX is the time in seconds
  - conductivity files (sigma__XXXX.0000000000.txt)
    - use bx utiliy to generate .exo file to plot in VisIt or Paraview

PFLOTRAN-E4D coupling

Option 1: PFLOTRAN built-in (current limitations)

- only Archie's law is implemented
- only PFLOTRAN rectangular grid is implemented (also no inactive cells)
- only passes fluid concentration, saturation, and temperature (if specified)
- runs in parallel
  - may not be efficient
  - needs 3 or more processors
  - hard to explore petrophysical relationships or fluid conductivities

PFLOTRAN-E4D coupling

Option 2: custom scripts

- Greater flexibility
  - use any output from any PFLOTRAN or other flow and transport models
  - explore petrophysical relationships or fluid conductivities
- **Solution:** use PFLOTRAN-E4D interpolation and mapping subroutines independently (needs compiling)
- Steps:
  1. Run PFLOTRAN
  2. Use a script to extract output from PFLOTRAN (in HDF5) and call the mapping subroutines to create E4D conductivities file
  3. Run E4D (forward model–mode 2)

Questions?

References I

T.C. Johnson, G. Hammond, X. Chen.

PFLOTRAN-E4D: A parallel open source PFLOTRAN module for simulating time-lapse electrical resistivity data, Computers and Geosciences 99:72–80, 2017.

PFLOTRAN documentation

PFLOTRAN documentation (hydrogeophysics mode)

E4D documentation

E4D current build

References II

- VisIt visualization software
- VisIt documentation

An example of using PFLOTRAN-E4D

Running PLOTRAN-E4D

example submission script

```
#!/bin/bash
#SBATCH --job-name=PFlotran
#SBATCH --output=slurm.out
#SBATCH --error=slurm.err
#SBATCH --workdir=/home/suhl/PFlotran/pflotran/example_problems/this_ex
#SBATCH -n 16
. /etc/profile.d/modules.sh   # load the module
module purge
# load the required modules  # note: 1-line
module load shared gcc/6.1.0 slurm/16.05.8 conda/2/4.3.21 hdf5/1.10.1
petsc/intel/gwil_mkl_3.9 intel/mkl/64/2017/1.132 intel/mpi/64/2017/1.132

export PATH=$PATH:/home/suhl/PFlotran/pflotran/src/pflotran/
mpirun -np 16 pflotran -pflotranin regional_doublet.in -num_slaves 4
```

List of input files

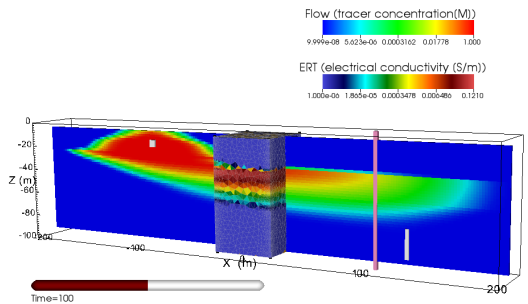
E4D files (*mode 1*), PFLOTRAN files, PFLOTRAN-E4D files

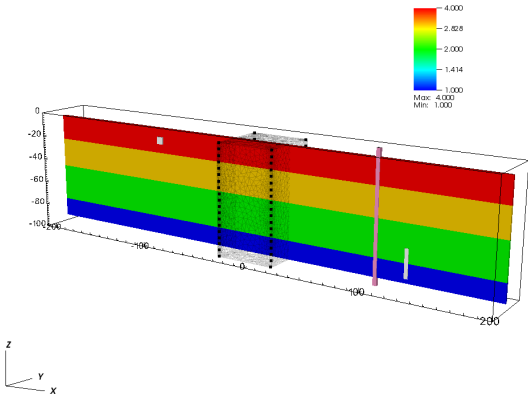
- archies.txt
- cmd2d.1.edge
- cmd2d.1.ele
- cmd2d.1.face
- cmd2d.1.neigh
- cmd2d.1.node
- *cmd2d.cfg*
- cmd2d.poly
- cmd2d.poly.1_orig.node
- cmd2d.sig
- cmd2d.srv
- cmd2d.trn
- *e4d.inp*
- list_file.txt
- mesh_build.log
- surface.1.node
- pf_mesh.txt
- regional_doublet.in
- surface.1.edge
- surface.1.ele
- surface.1.ele.old
- surface.1.neigh
- surface.1.poly
- surface.poly
- surface.sig

Note: "cmd2d" and "regional-doublet" are user-defined prefixes

Problem set-up

- 2D flow and transport: tracer migration left to right
- 3D ERT cell at centre





PFLOTRAN-E4D input files

e4d.inp

```
2                   E4D run mode
cmd2d.1.node        name of the mesh node file
cmd2d.srv           name of the baseline E4D survey file
cmd2d.sig           name of the baseline conductivity file
archies.txt         contains the archies paramters
list_file.txt       contains list of times to run E4D
```

archies.txt

```
129064                              Number of E4D cells
1.0000 1.3000 2.0000 0.0190
1.0000 1.3000 2.0000 0.0190
1.0000 1.3000 2.0000 0.0190


...   (repeat for each E4D cells)
```

- column 1: a = archies toruosity factor
- column 2: c = archies cementation factor
- column 3: m = archies saturation exponent
- column 4: t = temperature correction factor (if used)

list_file.txt

```
10                                  Number of times to call E4D
1728000.0000 cmd2d.srv cmd2d.sig
3456000.0000 cmd2d.srv cmd2d.sig
5184000.0000 cmd2d.srv cmd2d.sig
6912000.0000 cmd2d.srv cmd2d.sig
8640000.0000 cmd2d.srv cmd2d.sig
10368000.0000 cmd2d.srv cmd2d.sig
12096000.0000 cmd2d.srv cmd2d.sig
13824000.0000 cmd2d.srv cmd2d.sig
15552000.0000 cmd2d.srv cmd2d.sig
17280000.0000 cmd2d.srv cmd2d.sig

time(s),survey file (design must be same as baseline),
conductivity at this time
```

pf_mesh.txt

```
250                                  Number of PFLOTRAN cells in x
-250.0000 -248.0000 -246.0000 ...     Location of each node in x
1                                    Number of PFLOTRAN cells in y
-1.0000 1.0000                      Location of each node in y
60                                   Number of PFLOTRAN cells in z
-250.00 -220.00 -190.0000 ...        Location of each node in z
```

PFLOTRAN input file

PFLOTRAN input deck

- Very flexible: in blocks, order does not matter
- The input deck card is all inclusive, but can call data files if needed (very helpful for dynamic boundary conditions etc.)
- Can pretty much treat any property as time-varying

SIMULATION

- Specify subsurface simulation and Richards mode

```
SIMULATION
SIMULATION_TYPE   HYDROGEOPHYSICS  # use SUBSURFACE if PF only #
PROCESS_MODELS
SUBSURFACE_FLOW flow
MODE RICHARDS
/
SUBSURFACE_TRANSPORT transport
GLOBAL_IMPLICIT
/
/
/
END
SUBSURFACE
```

GRID

- Problem domain: $500 \times 1 \times 100$ m (x $\times$ y $\times$ z)
- Grid resolution $1 \times 1 \times 1$ m

```
GRID
TYPE STRUCTURED      ! structured grid
NXYZ 250 1 50         ! NX, NY, NZ
BOUNDS               ! define the rectangular domain
 -250.d0 -1.d0 -100.d0     ! xmin ymin zmin
250.d0 1.d0 0.d0    ! xmax ymax zmax
/
END
```

MATERIAL_PROPERTY

```
MATERIAL_PROPERTY soil1
ID 1
POROSITY 0.25d0
TORTUOSITY 0.5d0
CHARACTERISTIC_CURVES cc1
PERMEABILITY
PERM_X 5.d-9  ! option to define property cell-by-cell using a HDF5 file
PERM_Y 5.d-9
PERM_Z 5.d-10
/
END
```

repeate for all 4 materials

SATURATION FUNCTIONS

```
CHARACTERISTIC_CURVES cc1
SATURATION_FUNCTION VAN_GENUCHTEN
ALPHA  1.d-4
M 0.5d0
LIQUID_RESIDUAL_SATURATION 0.1d0
MAX_CAPILLARY_PRESSURE 1.d8
/
PERMEABILITY_FUNCTION MUALEM_VG_LIQ
M 0.5d0
LIQUID_RESIDUAL_SATURATION 0.1d0
/
END
```

FLUID_PROPERTY & CHEMISTRY

- Assign a molecular diffusion coefficient of 10^{-9} m^2/s to all aqueous species

```
FLUID_PROPERTY                    ! fluid is water
DIFFUSION_COEFFICIENT 1.d-9    ! [m2/s]
END  ! <-- closes out FLUID_PROPERTY card

CHEMISTRY
PRIMARY_SPECIES
Tracer  % Tracer must be a primary species when running PFLOTRAN-E4D
/
OUTPUT
TOTAL
all
/
END
```

REGION I

```
REGION all
COORDINATES
-250.d0 -1.d0    -100.d0
250.d0 1.d0 0.d0
/
END

REGION layer1
COORDINATES
-250.d0    -1.d0    -100.d0
250.d0 1.d0 -80.d0
/
END
(repeat for all layers)
```

REGION II

```
REGION west
COORDINATES
-250.d0 -1.d0    -100.d0
-250.d0 1.d0 0.d0
/
FACE WEST
END
(repeat for all faces that needs assigning B.C.)
```

REGION III

```
REGION injection_well
COORDINATES
-100.d0 0.d0 -16.d0
-100.d0 0.d0 -15.d0
/
END


REGION Obs_pt_center
COORDINATE 125.d0 0.d0 -40.d0
END
```

STRATA

- Couple soil1 rock/soil type with region 1 to define a stratigraphic unit
- Alternatively, you can define unit membership of each cell using a HDF5 file

```
STRATA
REGION layer1
MATERIAL soil1
END

STRATA
MATERIAL materials_and_region.h5 !script to convert from text file
END                                !available on pflotran.org
```

SATURATION FUNCTIONS

```
CHARACTERISTIC_CURVES cc1
SATURATION_FUNCTION VAN_GENUCHTEN
ALPHA  1.d-4
M 0.5d0
LIQUID_RESIDUAL_SATURATION 0.1d0
MAX_CAPILLARY_PRESSURE 1.d8
/
PERMEABILITY_FUNCTION MUALEM_VG_LIQ
M 0.5d0
LIQUID_RESIDUAL_SATURATION 0.1d0
/
END
```

INTEGRAL FLUX

- Mass discharge of solute across a user-defined plane (may have more than 1)

```
INTEGRAL_FLUX mass_flux
COORDINATES
100.d0 -1.d0 -100.d0
100.d0 1.d0 0.d0
/
/
```

FLOW_CONDITION I

- water table, injection, pumping etc.

```
FLOW_CONDITION initial
TYPE
PRESSURE HYDROSTATIC
/
INTERPOLATION LINEAR
DATUM 0.d0 0.d0 -30.d0  ! water table at z= -30 m..
GRADIENT
PRESSURE -0.002 0. 0.   ! gradient is dH/dz = -0.002
/
PRESSURE 101325.d0
END
```

FLOW_CONDITION II

```
FLOW_CONDITION injection
TYPE
RATE SCALED_VOLUMETRIC_RATE NEIGHBOR_PERM
/
RATE 5.08 m^3/day  ! injection rate is positive
END

FLOW_CONDITION extraction
TYPE
RATE SCALED_VOLUMETRIC_RATE NEIGHBOR_PERM
/
RATE -250 m^3/day ! pumping rate is negative
END
```

TRANSPORT_CONDITION (important!) I

- Couple transport constraints with transport conditions
- Tracer concentration is passed to E4D for fluid conductivity
- $1.0\,T = 1\ mol/m^3 = 1000\ \mu S/cm = 0.1\ S/m$

```
TRANSPORT_CONDITION initial  ! named initial...
TYPE DIRICHLET_ZERO_GRADIENT ! this is a zero gradient bc
CONSTRAINT initial ! name of constraint
CONCENTRATIONS
Tracer  1.d-2 T ! background groundwater concentration
/
/
END
TRANSPORT_CONDITION west
```

TRANSPORT_CONDITION (important!) II

```
TYPE DIRICHLET_ZERO_GRADIENT
CONSTRAINT west
CONCENTRATIONS
Tracer  1.d-2 T
/
/
END
```

```
TRANSPORT_CONDITION injection
TYPE DIRICHLET_ZERO_GRADIENT
CONSTRAINT injection
CONCENTRATIONS
Tracer  1.d0   T ! tracer concentration
/
/
END
```

CONDITION COUPLERS I

```
# initial condition
INITIAL_CONDITION % give a name
FLOW_CONDITION initial % choose a flow condition
TRANSPORT_CONDITION initial % choose a transport condition
REGION all % choose a region
END

# west boundary condition
BOUNDARY_CONDITION west
FLOW_CONDITION initial
TRANSPORT_CONDITION west
REGION west
END
```

CONDITION COUPLERS II

```
# source
SOURCE_SINK injection_well
FLOW_CONDITION injection
TRANSPORT_CONDITION injection
REGION injection_well
END

# sink
SOURCE_SINK extraction_well
FLOW_CONDITION extraction
TRANSPORT_CONDITION initial
REGION extraction_well
END
```

TIME

- Set final simulation time to 25 days
- Set initial time step size to 1.e-2 days
- Set maximum time step size to 5.0 days

```
TIME
FINAL_TIME 25.d0 d              ! Within TIME, time units
INITIAL_TIMESTEP_SIZE 1.d-2 d     ! are recognized and
MAXIMUM_TIMESTEP_SIZE 5d0 d   ! converted to SI
END                                 ! (i.e. y, h --> s).
```

OUTPUT

- Specify output times (5, 10, 15, 20 years) and format (Tecplot point datapacking and HDF5).
- The initial and final simulation times are automatically added to output
- Make sure output times include all the times you want to call E4D !

```
OUTPUT
SNAPSHOT_FILE  ! (below) I want every 20 d, even it stops at 200 d
    PERIODIC TIME 20. d between 0. y and 10. y
    # TIMES d 20. 40. 60. ! or you can specify one-by-one
FORMAT TECPLOT POINT
        FORMAT HDF5
        PRINT_COLUMN_IDS
            /
END
```

Summary

- High-level overview of coupled hydrogeophysical modelling
  - motivation
  - concepts for implementation
- Discussed specifics of PFLOTRAN-E4D
- Went through input files for PFLOTRAN-E4D
- How can you take advantage of coupled hydrogeophysical modelling for your problem?