PFLOTRAN-E4D-SIP Module Usage Description

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Required files within directory:

1. e4d input file
2. conductivity file
3. survey file
4. archies_tmp.txt
5. list_file.txt
6. pf_mesh.txt
7. e4d mesh files (all the accessory files)
8. PFLOTRAN input file (hydrogeophysics module)

INPUT FILES

E4D input files for SIP

The file e4d.inp is the main input file for the E4d module. E4D reads e4d.inp to identify the remaining files necessary to run E4D. The e4d.inp file must have 6 lines, as follows (note the e4d.inp file for the pflotran module has a different format than the e4d.inp file for the standalone, full version of E4D),

mesh_node_file	This is the name of the mesh node file
base_survey_file	This is the name of the baseline e4d survey file
conductivity_file	This is the name of the baseline conductivity file
archies_tmp.txt	This is for archies factor to interpolate PFLOTRAN to E4D
list_file	This is the name of the survey listing file
e4d.out	This is equivalent to output file of e4d

*e4d.out is not required during **PFLOTRAN-E4D** simulation

Archies_tmp.txt

The archies_tmp.txt file should be on the fourth line of e4d.inp file. This file consist four factors data for each element. Four factors are tortuosity factor, cementation factor, saturation exponent, and temperature correction factor. File format is as follows:

Total_element_number_in_e4d_mesh
Tortuosity_factor1 cementation_factor1 saturation_exponent1, temperature_correction_factor1
.
.
.
.
Tortuosity_factor* cementation_factor* saturation_exponent*, temperature_correction_factor*

list_file.txt

The list file name is specified on the fifth line of e4d.inp. The list file tells the E4D module at which times ERT surveys should be simulated. For each time specified, it lists a conductivity file and a survey file. The conductivity file specified for a given time is used to tell E4D what bulk conductivity values should be used for regions that are outside of the PFLOTRAN domain, and therefore have no interpolated values from PFLOTRAN. The survey file specified at each time is used to provide observed measurements values, which are repeated in the output files, primarily as an aid for joint

inversions. Each survey file must have the same format and measurement sequence as the baseline survey file. The only value that is allowed to be different is the observed measurement V/I and standard deviation.

The list file also specifies parameters used in the petrophysical transform. The format of the list file is as follows:

```
NT     FF     FC_sw          FC_gw
t1     surv_1  cond_1
t2     surv_2  cond_2
.
.
.
tNT    surv_NT cond_NT
```

where:
NT = number of times to simulate ERT surveys
FF = Formation Factor (used in the petro. transform)
FC_sw = surface water fluid conductivity (used in the petro. transform)
FC-gw = groundwater fluid conductivity (used in the current petro. transform)
tx = time x to compute ERT survey(must be specified exactly in PFLOTRAN time)
surv_x = survey file for time x.
cond_x = conductivity file for time x.

Regions of the ERT domain that are outside of the PFLOTRAN domain will assume the values specified in file cond_x file at time x.

The the conductivity and survey files specified in the list file need not be unique. The same file(s) may be specified for more than once. This is the most common use.

pf_mesh.txt
In order to interpolate PFLOTRAN states to the E4D mesh, E4D must know the PFLOTRAN mesh dimensions. PFLOTRAN currently does not provide it's mesh dimensions to E4D, so they must be specified in an input file. The input file where the PFLOTRAN mesh dimensions are provided is pf_mesh.txt. The format of pf_mesh is as follows:

```
ncx
nx_1   nx_2  ...  nx_ncx+1

ncy
ny_1   ny_2  ...  ny_ncy+1

ncz
nz_1   nz_2  ...  nz_ncz+1
```

where:

ncx is the number of cells in the x dimension
nx_* is the *th node position in the x direction. Note there are ncx+1 node postions for ncx cells.

The blocks starting with ncy and ncz are analogous to the ncx block specified above.
Updated by Bulbul: If model has x cells and then it will have x+1 nodes. nx_*, ny_*, and nz_* will start from minimum value and finish at maximum value. nx_*, ny_*, and nz_*, each of them should be in one line no punctuation (i.e., \) is allowed.

OUTPUT FILES
conductivity files
E4D writes a simulated bulk conductivity file for each time step specified in the list file. The format of the conductivity file is that same as in the full version of E4D. The name of the file is each time step is sigma_Rx*.txt, where x is the realization number, and * is the time stamp specified in the list file.

simulated and observed data file
E4D writes the simulated and observed ERT measurements to a file for each time step specified in the list file. For each time step, the file name is E4D_x*.txt, where x is the realization number and * is the time stamp specified in the list file.

CALLING SEQUENCE
The plflotran input file have the SIMULATION_TYPE HYDROGEOPHYSICS flag. See pflotran documentation for details. The command line sequence to run PFLOTRAN with the E4D module is:

mpirun -n TP pflotran -pflotranin PFIN < -stochastic > < -num_realizations NR >
< -num_groups NG> -num_slaves NS

where:
TP = total number of process (i.e. compute cores) to use
PFIN = pflotran input file name
NR = number of realizations to generate in stochastic mode
NG = number of execution groups to use when running in stochastic mode
NS = number of E4D slaves processes to use. In total, E4D will use NS+1 processes, one for the master process and NS slave processes. NS should not exceed the number of electrodes specified in the electrode block of the survey file, or else E4D will terminate.

0ptions in <> are only used in stochastic mode. If stochastic mode is used, the number of processes allocated to E4D is NG*(NS+1). The remainder of the processes are allocated to PFLOTRAN, with (TP-NG(NS+1))/NG processes per group.

Real command:

mpirun -n 60 $PFLOTRAN_DIR/src/pflotran/pflotran -pflotranin mypflotran.in -num_realizations 1 -num_slaves 41 -num_groups 1 –stochastic

We have wrote a python script that populate factors and SIP data for each element based on zones. The code requires a factor (to create archies_tmp.txt fiel) or sigdata (to create SIP conductivity file) file to read for each zone of the E4D mesh. Header is necessary on the file although it is ignored while it is read. The script read the given file and populate the data on each element of the mesh. The name of the script is get_archies_params.py.