pestpp-opt

May 1, 2019

1 Run PESTPP-OPT

In [1]:
```
import os
import shutil
import numpy as np
import pandas as pd
import matplotlib.pyplot as plt
import flopy
import pyemu
```

```
flopy is installed in /Users/jeremyw/Dev/gw1876/activities_2day_mfm/notebooks/flopy
```

In [2]:
```
t_d = "template"
m_d = "master_opt"
```

In [3]:
```
pst = pyemu.Pst(os.path.join(t_d,"freyberg.pst"))
pst.write_par_summary_table(filename="none").sort_index()
```

Out[3]:

	type	transform	count	initial value	\
cn_hk6	cn_hk6	log	1	0	
cn_hk7	cn_hk7	log	1	0	
cn_hk8	cn_hk8	log	1	0	
cn_prsity6	cn_prsity6	log	1	0	
cn_prsity7	cn_prsity7	log	1	0	
cn_prsity8	cn_prsity8	log	1	0	
cn_rech4	cn_rech4	log	1	0	
cn_rech5	cn_rech5	log	1	-0.39794	
cn_ss6	cn_ss6	log	1	0	
cn_ss7	cn_ss7	log	1	0	
cn_ss8	cn_ss8	log	1	0	
cn_strt6	cn_strt6	log	1	0	
cn_strt7	cn_strt7	log	1	0	
cn_strt8	cn_strt8	log	1	0	
cn_sy6	cn_sy6	log	1	0	
cn_sy7	cn_sy7	log	1	0	
cn_sy8	cn_sy8	log	1	0	

cn_vka6	cn_vka6	log	1	0
cn_vka7	cn_vka7	log	1	0
cn_vka8	cn_vka8	log	1	0
drncond_k00	drncond_k00	log	10	0
flow	flow	log	1	0
gr_hk3	gr_hk3	log	705	0
gr_hk4	gr_hk4	log	705	0
gr_hk5	gr_hk5	log	705	0
gr_prsity3	gr_prsity3	log	705	0
gr_prsity4	gr_prsity4	log	705	0
gr_prsity5	gr_prsity5	log	705	0
gr_rech2	gr_rech2	log	705	0
gr_rech3	gr_rech3	log	705	0
...	...	...	...	...
gr_strt5	gr_strt5	log	705	0
gr_sy3	gr_sy3	log	705	0
gr_sy4	gr_sy4	log	705	0
gr_sy5	gr_sy5	log	705	0
gr_vka3	gr_vka3	log	705	0
gr_vka4	gr_vka4	log	705	0
gr_vka5	gr_vka5	log	705	0
pp_hk0	pp_hk0	log	32	0
pp_hk1	pp_hk1	log	32	0
pp_hk2	pp_hk2	log	32	0
pp_prsity0	pp_prsity0	log	32	0
pp_prsity1	pp_prsity1	log	32	0
pp_prsity2	pp_prsity2	log	32	0
pp_rech0	pp_rech0	log	32	0
pp_rech1	pp_rech1	log	32	0
pp_ss0	pp_ss0	log	32	0
pp_ss1	pp_ss1	log	32	0
pp_ss2	pp_ss2	log	32	0
pp_strt0	pp_strt0	log	32	0
pp_strt1	pp_strt1	log	32	0
pp_strt2	pp_strt2	log	32	0
pp_sy0	pp_sy0	log	32	0
pp_sy1	pp_sy1	log	32	0
pp_sy2	pp_sy2	log	32	0
pp_vka0	pp_vka0	log	32	0
pp_vka1	pp_vka1	log	32	0
pp_vka2	pp_vka2	log	32	0
strk	strk	log	40	0
welflux	welflux	log	2	0 to 0.176091
welflux_k02	welflux_k02	log	6	0

	upper bound	lower bound	standard deviation
cn_hk6	1	-1	0.5
cn_hk7	1	-1	0.5

cn_hk8	1	-1	0.5
cn_prsity6	0	-1	0.25
cn_prsity7	0	-1	0.25
cn_prsity8	0	-1	0.25
cn_rech4	0.0791812	-0.09691	0.0440228
cn_rech5	-0.09691	-1	0.225772
cn_ss6	1	-1	0.5
cn_ss7	1	-1	0.5
cn_ss8	1	-1	0.5
cn_strt6	0.0211893	-0.0222764	0.0108664
cn_strt7	0.0211893	-0.0222764	0.0108664
cn_strt8	0.0211893	-0.0222764	0.0108664
cn_sy6	0.243038	-0.60206	0.211275
cn_sy7	0.243038	-0.60206	0.211275
cn_sy8	0.243038	-0.60206	0.211275
cn_vka6	1	-1	0.5
cn_vka7	1	-1	0.5
cn_vka8	1	-1	0.5
drncond_k00	1	-1	0.5
flow	0.09691	-0.124939	0.0554622
gr_hk3	1	-1	0.5
gr_hk4	1	-1	0.5
gr_hk5	1	-1	0.5
gr_prsity3	0	-1	0.25
gr_prsity4	0	-1	0.25
gr_prsity5	0	-1	0.25
gr_rech2	0.0413927	-0.0457575	0.0217875
gr_rech3	0.0413927	-0.0457575	0.0217875
...	...	...	...
gr_strt5	0.0211893	-0.0222764	0.0108664
gr_sy3	0.243038	-0.60206	0.211275
gr_sy4	0.243038	-0.60206	0.211275
gr_sy5	0.243038	-0.60206	0.211275
gr_vka3	1	-1	0.5
gr_vka4	1	-1	0.5
gr_vka5	1	-1	0.5
pp_hk0	1	-1	0.5
pp_hk1	1	-1	0.5
pp_hk2	1	-1	0.5
pp_prsity0	0	-1	0.25
pp_prsity1	0	-1	0.25
pp_prsity2	0	-1	0.25
pp_rech0	0.0413927	-0.0457575	0.0217875
pp_rech1	0.0413927	-0.0457575	0.0217875
pp_ss0	1	-1	0.5
pp_ss1	1	-1	0.5
pp_ss2	1	-1	0.5
pp_strt0	0.0211893	-0.0222764	0.0108664

```
pp_strt1                0.0211893         -0.0222764              0.0108664
pp_strt2                0.0211893         -0.0222764              0.0108664
pp_sy0                   0.243038           -0.60206               0.211275
pp_sy1                   0.243038           -0.60206               0.211275
pp_sy2                   0.243038           -0.60206               0.211275
pp_vka0                         1                 -1                    0.5
pp_vka1                         1                 -1                    0.5
pp_vka2                         1                 -1                    0.5
strk                            2                 -2                      1
welflux      0.176091 to 0.30103  -0.30103 to      0  0.0752575 to 0.11928
welflux_k02                     1                 -1                    0.5

[65 rows x 7 columns]
```

In [4]:
```
pst.pestpp_options = {}
#dvg = ["welflux_k02","welflux"]
dvg = ["welflux_k02"]
pst.pestpp_options["opt_dec_var_groups"] = dvg
pst.pestpp_options["opt_direction"] = "max"
```

In [5]:
```
par = pst.parameter_data
par.loc[:,"partrans"] = "fixed"

#turn off pumping in the scenario
par.loc["welflux_001","parlbnd"] = 0.0
par.loc["welflux_001","parval1"] = 0.0
dvg_pars = par.loc[par.pargp.apply(lambda x: x in dvg),"parnme"]
par.loc[dvg_pars,"partrans"] = "none"
par.loc[dvg_pars,"parlbnd"] = 0.0
par.loc[dvg_pars,"parubnd"] = 2.0
par.loc[dvg_pars,"parval1"] = 1.0

pst.rectify_pgroups()
pst.parameter_groups.loc[dvg,"inctyp"] = "absolute"
pst.parameter_groups.loc[dvg,"inctyp"] = "absolute"
pst.parameter_groups.loc[dvg,"derinc"] = 0.25

pst.parameter_groups.loc[dvg,:]
```

Out[5]:
```
                pargpnme    inctyp  derinc  derinclb  forcen  derincmul  \
pargpnme
welflux_k02  welflux_k02  absolute    0.25       0.0  switch        2.0

               dermthd  splitthresh  splitreldiff splitaction  extra
pargpnme
welflux_k02  parabolic      0.00001           0.5     smaller    NaN
```

1.0.1 constraints

```
In [6]: obs = pst.observation_data
        obs.loc[:,"weight"] = 0.0
        swgw_hist = obs.loc[obs.obsnme.apply(lambda x: "fa" in x and( "hw" in x or "tw" in x))
        obs.loc[swgw_hist,:]
```

Out[6]:

	obsnme	obsval	weight	obgnme	extra
obsnme					
fa_hw_19791230	fa_hw_19791230	-1283.91010	0.0	flaqx	NaN
fa_hw_19801229	fa_hw_19801229	-747.97600	0.0	flaqx	NaN
fa_tw_19791230	fa_tw_19791230	-589.80970	0.0	flaqx	NaN
fa_tw_19801229	fa_tw_19801229	-214.77211	0.0	flaqx	NaN

We need to change the obs group (obgnme) so that pestpp-opt will recognize these two model outputs as constraints. lets also assume that the sw-gw flux needs to be at least -1000

```
In [7]: obs.loc[swgw_hist,"obgnme"] = "less_than"
        obs.loc[swgw_hist,"weight"] = 1.0

        obs.loc[swgw_hist,"obsval"] = -300

        tot_abs_rate = ["flx_wells_19791230"]#,"flx_wells_19801229"]
        obs.loc[tot_abs_rate,"obgnme"] = "less_than"
        obs.loc[tot_abs_rate,"weight"] = 1.0
        obs.loc[tot_abs_rate,"obsval"] = -600.0
        pst.less_than_obs_constraints
```

```
Out[7]: obsnme
        fa_hw_19791230           fa_hw_19791230
        fa_hw_19801229           fa_hw_19801229
        fa_tw_19791230           fa_tw_19791230
        fa_tw_19801229           fa_tw_19801229
        flx_wells_19791230    flx_wells_19791230
        Name: obsnme, dtype: object
```

```
In [8]: pst.control_data.noptmax = 1
        pst.write(os.path.join(t_d,"freyberg_opt.pst"))
```

```
In [9]: pyemu.os_utils.start_slaves(t_d,"pestpp-opt","freyberg_opt.pst",num_slaves=10,master_di
```

```
In [10]: jco = pyemu.Jco.from_binary(os.path.join(m_d,"freyberg_opt.1.jcb")).to_dataframe().loc
         jco
```

Out[10]:

	wf0200090016	wf0200110013	wf0200200014	wf0200260010	\
fa_hw_19791230	137.57200	126.32400	46.30000	21.90800	
fa_hw_19801229	22.58400	28.65600	12.03600	12.29200	
fa_tw_19791230	6.50728	14.53516	93.28136	92.42320	
fa_tw_19801229	4.10836	7.60104	15.29948	30.88604	

```
flx_wells_19791230    -150.00000    -150.00000    -150.00000    -150.00000

                      wf0200290006  wf0200340012
fa_hw_19791230           18.12000       4.8320
fa_hw_19801229           13.12800       3.3560
fa_tw_19791230           71.84608      82.9612
fa_tw_19801229           34.79872      17.5232
flx_wells_19791230     -150.00000    -150.0000
```

In [11]:
```
par_df = pyemu.pst_utils.read_parfile(os.path.join(m_d,"freyberg_opt.1.par"))
print(par_df.loc[dvg_pars,"parval1"].sum())
par_df.loc[dvg_pars,:]
```

```
8.1332977617072
```

Out[11]:

	parnme	parval1	scale	offset
parnme				
wf0200090016	wf0200090016	2.000000	1.0	0.0
wf0200110013	wf0200110013	2.000000	1.0	0.0
wf0200200014	wf0200200014	2.000000	1.0	0.0
wf0200260010	wf0200260010	0.133298	1.0	0.0
wf0200290006	wf0200290006	0.000000	1.0	0.0
wf0200340012	wf0200340012	2.000000	1.0	0.0

In [12]:
```
pst = pyemu.Pst(os.path.join(m_d,"freyberg_opt.pst"),resfile=os.path.join(m_d,"freybe
pst.res.loc[pst.nnz_obs_names,:]
```

Out[12]:

	name	group	measured	modelled	\
name					
fa_hw_19791230	fa_hw_19791230	less_than	-300.0	-699.3735	
fa_hw_19801229	fa_hw_19801229	less_than	-300.0	-714.4580	
fa_tw_19791230	fa_tw_19791230	less_than	-300.0	-407.7249	
fa_tw_19801229	fa_tw_19801229	less_than	-300.0	-299.7868	
flx_wells_19791230	flx_wells_19791230	less_than	-600.0	-1219.9948	

	residual	weight
name		
fa_hw_19791230	399.3735	1.0
fa_hw_19801229	414.4580	1.0
fa_tw_19791230	107.7249	1.0
fa_tw_19801229	-0.2132	1.0
flx_wells_19791230	619.9948	1.0

In [13]:
```
#todo chance constraints (fosm and en-based), well pars and constraints in scen perio
```

1.0.2 Opt under uncertainty part 1: FOSM chance constraints

In [14]:
```
pst.pestpp_options["opt_risk"] = 0.4
```

In [15]:
```
cn_pars = par.loc[par.pargp.apply(lambda x: "cn" in x),"parnme"]
cn_pars
```

Out[15]:
```
parnme
hk6_cn            hk6_cn
hk7_cn            hk7_cn
hk8_cn            hk8_cn
prsity6_cn    prsity6_cn
prsity7_cn    prsity7_cn
prsity8_cn    prsity8_cn
rech4_cn        rech4_cn
rech5_cn        rech5_cn
ss6_cn            ss6_cn
ss7_cn            ss7_cn
ss8_cn            ss8_cn
strt6_cn        strt6_cn
strt7_cn        strt7_cn
strt8_cn        strt8_cn
sy6_cn            sy6_cn
sy7_cn            sy7_cn
sy8_cn            sy8_cn
vka6_cn          vka6_cn
vka7_cn          vka7_cn
vka8_cn          vka8_cn
Name: parnme, dtype: object
```

In [16]:
```
par = pst.parameter_data
par.loc[cn_pars,"partrans"] = "log"
pst.control_data.noptmax = 1
pst.write(os.path.join(t_d,"freyberg_opt_uu1.pst"))
pst.npar_adj
```

Out[16]:
```
26
```

In [17]:
```
pyemu.os_utils.start_slaves(t_d,"pestpp-opt","freyberg_opt_uu1.pst",num_slaves=20,mast
```

In [18]:
```
pst = pyemu.Pst(os.path.join(m_d,"freyberg_opt_uu1.pst"),resfile=os.path.join(m_d,"fre
pst.res.loc[pst.nnz_obs_names,:]
```

Out[18]:
```
                                   name      group  measured    modelled  \
name
fa_hw_19791230          fa_hw_19791230  less_than    -300.0  -666.13442
fa_hw_19801229          fa_hw_19801229  less_than    -300.0  -682.60800
fa_tw_19791230          fa_tw_19791230  less_than    -300.0  -223.47050
fa_tw_19801229          fa_tw_19801229  less_than    -300.0  -208.37540
flx_wells_19791230  flx_wells_19791230  less_than    -600.0 -1586.33800

                     residual  weight
name
```

```
fa_hw_19791230      366.13442     1.0
fa_hw_19801229      382.60800     1.0
fa_tw_19791230      -76.52950     1.0
fa_tw_19801229      -91.62460     1.0
flx_wells_19791230  986.33800     1.0
```

In [19]:
```
par_df = pyemu.pst_utils.read_parfile(os.path.join(m_d,"freyberg_opt_uu1.1.par"))
print(par_df.loc[dvg_pars,"parval1"].sum())
par_df.loc[dvg_pars,:]
```

```
10.575587155980312
```

Out[19]:

	parnme	parval1	scale	offset
parnme				
wf0200090016	wf0200090016	2.000000	1.0	0.0
wf0200110013	wf0200110013	2.000000	1.0	0.0
wf0200200014	wf0200200014	1.481006	1.0	0.0
wf0200260010	wf0200260010	1.094581	1.0	0.0
wf0200290006	wf0200290006	2.000000	1.0	0.0
wf0200340012	wf0200340012	2.000000	1.0	0.0

1.0.3 Opt under uncertainty part 2: ensemble-based chance constraints

In [20]:
```
obs_df = pd.read_csv(os.path.join("master_prior_sweep","sweep_out.csv"),index_col=0)
obs_df = obs_df.loc[obs_df.failed_flag==0,:]
```

In [21]:
```
std = obs_df.std().loc[pst.nnz_obs_names]
std
```

Out[21]:
```
fa_hw_19791230      393.163932
fa_hw_19801229      520.045334
fa_tw_19791230      488.802498
fa_tw_19801229      557.509594
flx_wells_19791230  756.211197
dtype: float64
```

In [22]:
```
pst.observation_data.loc[pst.nnz_obs_names,"weight"] = std.loc[pst.nnz_obs_names]
pst.pestpp_options["opt_std_weights"] = True
pst.write(os.path.join(t_d,"freyberg_opt_uu2.pst"))
```

In [23]:
```
pyemu.os_utils.start_slaves(t_d,"pestpp-opt","freyberg_opt_uu2.pst",num_slaves=10,mast
```

In [24]:
```
par_df = pyemu.pst_utils.read_parfile(os.path.join(m_d,"freyberg_opt_uu2.1.par"))
print(par_df.loc[dvg_pars,"parval1"].sum())
par_df.loc[dvg_pars,:]
```

```
11.092194313981116
```

Out[24]:

	parnme	parval1	scale	offset
parnme				
wf0200090016	wf0200090016	2.000000	1.0	0.0
wf0200110013	wf0200110013	2.000000	1.0	0.0
wf0200200014	wf0200200014	1.092194	1.0	0.0
wf0200260010	wf0200260010	2.000000	1.0	0.0
wf0200290006	wf0200290006	2.000000	1.0	0.0
wf0200340012	wf0200340012	2.000000	1.0	0.0