pestpp-opt

May 14, 2019

1 Run PESTPP-OPT

In this notebook we will setup and solve a mgmt optimization problem around how much groundwater can be pumped while maintaining sw-gw exchange

```
In [1]: import os
        import shutil
        import numpy as np
        import pandas as pd
        import matplotlib.pyplot as plt
        import matplotlib as mpl
        plt.rcParams['font.size']=12
        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	0.176091	-0.30103	0.11928
cn_prsity7	0.176091	-0.30103	0.11928
cn_prsity8	0.176091	-0.30103	0.11928
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	0.176091	-0.30103	0.11928
gr_prsity4	0.176091	-0.30103	0.11928
gr_prsity5	0.176091	-0.30103	0.11928
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	0.176091	-0.30103	0.11928
pp_prsity1	0.176091	-0.30103	0.11928
pp_prsity2	0.176091	-0.30103	0.11928
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]
```

define our decision varible group and also set some ++args. Conceptually, we are going to optimize current pumping rates to make sure we meet ecological flows under both historic (current) conditions and scenario (future) conditions. Remember the scenario is an extreme 1-year drought so if we pump too much now, the system will be too low to provide critical flows if next year is an extreme drough - transient memory!

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"
```

For the first run, we wont use chance constraints, so just fix all non-decision-variable parameter. We also need to set some realistic bounds on the `welflux` multiplier decision variables. Finally, we need to specify a larger derivative increment for the decision varible group

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"] = 3.0
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 define constraints

model-based and prior information constraints are identified in pestpp-opt by an obs group that starts with "less_than" or "greater_than" and a weight greater than zero. So first, we turn off all of the weights and get names for the sw-gw exchange forecasts (funny how optimization turns forecasts into constraints...)

In [6]:

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

Out[6]:

```
                          obsnme      obsval  weight obgnme  extra
obsnme
fa_hw_19791230  fa_hw_19791230 -1165.19711     0.0  flaqx    NaN
fa_hw_19801229  fa_hw_19801229  -154.89106     0.0  flaqx    NaN
fa_tw_19791230  fa_tw_19791230  -505.49290     0.0  flaqx    NaN
fa_tw_19801229  fa_tw_19801229    38.58960     0.0  flaqx    NaN
```

We need to change the obs group (obgnme) so that pestpp-opt will recognize these two model outputs as constraints. The obsval becomes the RHS of the constraint. We also need to set a lower bound constraint on the total abstraction rate (good thing we included all those list file budget components as observations!)

In [7]:

```
obs.loc[swgw_const,"obgnme"] = "less_than"
obs.loc[swgw_const,"weight"] = 1.0

# we must have at least 300 m3/day of flux from gw to sw
# for historic and scenario periods
# and for both headwaters and tailwaters
obs.loc[swgw_const,"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"] = -900.0
# pst.less_than_obs_constraints
```

Now we need to define a minimum total pumping rate, otherwise this opt problem might yield a solution that doesn't give enough water for the intended usage. We will do this through a prior information constraint since this just a sum of decision varible values - the required minimum value will the sum of current pumping rates:

```
In [8]: pyemu.pst_utils.pst_config["prior_fieldnames"]
```

```
Out[8]: ['pilbl', 'equation', 'weight', 'obgnme']
```

Since all pumping well are using the same rate, we can just use a `1.0` multiplier in front of each `wel.flux` decision varialbe. If that is not the case, then you need to set the multipliers to be more meaningful

```
In [9]: pi = pst.null_prior
        pi.loc["pi_1","obgnme"] = "greater_than"
        pi.loc["pi_1","pilbl"] = "pi_1"
        pi.loc["pi_1","equation"] = " + ".join(["1.0 * {0}".format(d) for d in dvg_pars]) +\
                                    " = {0}".format(par.loc[dvg_pars,"parval1"].sum())
        pi.loc["pi_1","weight"] = 1.0
        pi.equation["pi_1"]
```

```
Out[9]: '1.0 * wf0200090016 + 1.0 * wf0200110013 + 1.0 * wf0200200014 + 1.0 * wf0200260010 + 1
```

```
In [10]: pst.prior_information
```

```
Out[10]:              obgnme pilbl  \
         pi_1  greater_than  pi_1


         pi_1  1.0 * wf0200090016 + 1.0 * wf0200110013 + 1.0 * wf0200200014 + 1.0 * wf0200260

               weight
         pi_1     1.0
```

```
In [11]: pst.control_data.noptmax = 1
         pst.write(os.path.join(t_d,"freyberg_opt.pst"))
         pyemu.os_utils.start_slaves(t_d,"pestpp-opt","freyberg_opt.pst",num_slaves=10,master_

noptmax:1, npar_adj:6, nnz_obs:4
```

Let's load and inspect the response matrix

```
In [12]: jco = pyemu.Jco.from_binary(os.path.join(m_d,"freyberg_opt.1.jcb")).to_dataframe().lo
         jco
```

```
Out[12]:                 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

                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
```

We see the transient effects in the nonzero value between current pumping rates (columns) and scenario sw-gw exchange (rows from 1980)

Let's also load the optimal decision variable values:

```
In [13]: 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,:]
```

```
9.693626734842857
```

```
Out[13]:                    parnme   parval1  scale  offset
         parnme
         wf0200090016  wf0200090016  3.000000    1.0     0.0
         wf0200110013  wf0200110013  3.000000    1.0     0.0
         wf0200200014  wf0200200014  3.000000    1.0     0.0
         wf0200260010  wf0200260010  0.000000    1.0     0.0
         wf0200290006  wf0200290006  0.000000    1.0     0.0
         wf0200340012  wf0200340012  0.693627    1.0     0.0
```

The sum of these values is the optimal objective function value. However, since these are just mulitpliers on the pumping rate, this number isnt too meaningful. Instead, lets look at the residuals file

```
In [14]: 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[14]:                          name      group  measured  modelled  residual  \
         name
         fa_hw_19791230  fa_hw_19791230  less_than    -300.0 -398.5755   98.5755
         fa_hw_19801229  fa_hw_19801229  less_than    -300.0 -656.8370  356.8370
         fa_tw_19791230  fa_tw_19791230  less_than    -300.0 -414.1347  114.1347
         fa_tw_19801229  fa_tw_19801229  less_than    -300.0 -299.5820   -0.4180

                         weight
         name
         fa_hw_19791230     1.0
         fa_hw_19801229     1.0
         fa_tw_19791230     1.0
         fa_tw_19801229     1.0
```

Sweet as! lots of room in the optimization problem. The bounding constraint is the one closest to its RHS

1.0.2 Opt under uncertainty part 1: FOSM chance constraints

This is where the process of uncertainty quantification/history matching and mgmt optimizatiom meet - worlds collide!

Mechanically, in PESTPP-OPT, to activate the chance constraint process, we need to specific a risk != 0.5. Risk ranges from 0.001 (risk tolerant) to 0.999 (risk averse). The larger the risk value, the more confidence we have that the (uncertain) model-based constraints are truely satisfied. Here we will start with a risk tolerant stance:

```
In [15]: pst.pestpp_options["opt_risk"] = 0.4
```

For the FOSM-based chance constraints, we also need to have at least one adjustable non-dec-var parameter so that we can propogate parameter uncertainty to model-based constraints (this can also be posterior FOSM is non-constraint, non-zero-weight observations are specified). For this simple demo, lets just use the constant multiplier parameters in the prior uncertainty stance:

```
In [16]: cn_pars = par.loc[par.pargp.apply(lambda x: "cn" in x),"parnme"]
         cn_pars
```

```
Out[16]: 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 [17]: 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"))
```

```
noptmax:1, npar_adj:26, nnz_obs:4
```

So now we need to not only fill the response matrix (between dec vars and constraints) but we also need to fill the jacobian matrix (between parameters and constraints).

```
In [18]: pyemu.os_utils.start_slaves(t_d,"pestpp-opt","freyberg_opt_uu1.pst",num_slaves=20,mas
```

```
In [19]: 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[19]:                          name      group  measured  modelled  residual  \
         name
         fa_hw_19791230  fa_hw_19791230  less_than    -300.0 -426.6231  126.6231
         fa_hw_19801229  fa_hw_19801229  less_than    -300.0 -640.6620  340.6620
         fa_tw_19791230  fa_tw_19791230  less_than    -300.0 -223.3317  -76.6683
         fa_tw_19801229  fa_tw_19801229  less_than    -300.0 -208.3292  -91.6708

                         weight
         name
         fa_hw_19791230     1.0
         fa_hw_19801229     1.0
         fa_tw_19791230     1.0
         fa_tw_19801229     1.0
```

```
In [20]: 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,:]
```

```
12.500896512450069
```

```
Out[20]:                    parnme   parval1  scale  offset
         parnme
         wf0200090016  wf0200090016  3.000000    1.0     0.0
         wf0200110013  wf0200110013  3.000000    1.0     0.0
         wf0200200014  wf0200200014  1.281895    1.0     0.0
         wf0200260010  wf0200260010  0.000000    1.0     0.0
         wf0200290006  wf0200290006  2.219002    1.0     0.0
         wf0200340012  wf0200340012  3.000000    1.0     0.0
```

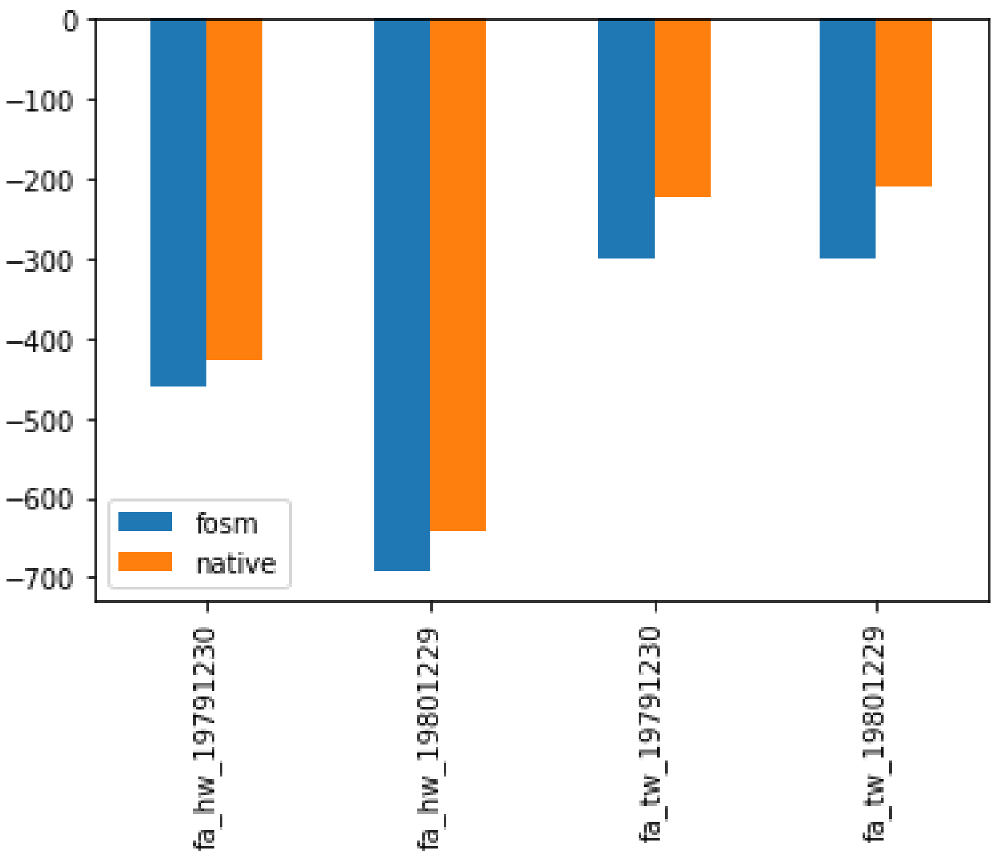
We now see how taking a risk tolerant stance allows for more pumping but that we have only a 40% chance of actually satifying the sw-gw constraints (see how the model simulated value is actually in violation of the -300 constraint RHS. Lets check the residuals that include the FOSM-based chance constraint shift:

```
In [21]: res_df = pyemu.pst_utils.read_resfile(os.path.join(m_d,"freyberg_opt_uu1.1.sim+fosm.re
         res_df
```

```
Out[21]:                          name      group  measured    modelled    residual  \
         name
         fa_hw_19791230  fa_hw_19791230  less_than    -300.0 -461.842970  161.842970
```

```
fa_hw_19801229  fa_hw_19801229  less_than    -300.0 -693.498392  393.498392
fa_tw_19791230  fa_tw_19791230  less_than    -300.0 -299.758707   -0.241293
fa_tw_19801229  fa_tw_19801229  less_than    -300.0 -299.676541   -0.323459

                weight
name
fa_hw_19791230     1.0
fa_hw_19801229     1.0
fa_tw_19791230     1.0
fa_tw_19801229     1.0
```

In [22]:
```
ax = pd.DataFrame({"native":pst.res.modelled,"fosm":res_df.modelled}).loc[pst.nnz_obs_
```



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

PESTPP-OPT can also skip the FOSM calculations if users specify model-based constraint weights as standard deviations (e.g. uncertainty in the forecasts/constraints). These can be derived from existing ensembles (oh snap!)

In [23]:
```
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 [24]: pr_std = obs_df.std().loc[pst.nnz_obs_names]
         pr_std
```

```
Out[24]: fa_hw_19791230    352.032747
         fa_hw_19801229    481.036378
         fa_tw_19791230    480.732852
         fa_tw_19801229    571.599106
         dtype: float64
```

```
In [25]: pst.observation_data.loc[pst.nnz_obs_names,"weight"] = pr_std.loc[pst.nnz_obs_names]
         pst.pestpp_options["opt_std_weights"] = True
         pst.write(os.path.join(t_d,"freyberg_opt_uu2.pst"))
```

```
noptmax:1, npar_adj:26, nnz_obs:4
```

```
In [26]: pyemu.os_utils.start_slaves(t_d,"pestpp-opt","freyberg_opt_uu2.pst",num_slaves=10,mas
```

```
In [27]: 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,:]
```

```
13.177556909488672
```

Out[27]:

parnme	parnme	parval1	scale	offset
wf0200090016	wf0200090016	3.000000	1.0	0.0
wf0200110013	wf0200110013	3.000000	1.0	0.0
wf0200200014	wf0200200014	0.000000	1.0	0.0
wf0200260010	wf0200260010	1.177557	1.0	0.0
wf0200290006	wf0200290006	3.000000	1.0	0.0
wf0200340012	wf0200340012	3.000000	1.0	0.0

Why is the objective function higher when we use the ensemble-based constraint uncertainty compared to the FOSM constraint uncertainty? remember how many more parameters were used in the ensemble analyses compared to just the hand full of constant by layer parameters???

1.0.4 Super secret mode

turns out, if the opt problem is truely linear, we can reuse results of a previous PESTPP-OPT run to modify lots of the pieces of the optimization problem and resolve the optimization problem without running the model even once! WAT!? This is done by specifying some additional ++ args (and copying some files around)

```
In [28]: shutil.copy2(os.path.join(m_d,"freyberg_opt_uu2.1.jcb"),os.path.join(m_d,"restart.jcb
         shutil.copy2(os.path.join(m_d,"freyberg_opt_uu2.1.jcb.rei"),os.path.join(m_d,"restart

         pst.pestpp_options["base_jacobian"] = "restart.jcb"
         pst.pestpp_options["hotstart_resfile"] = "restart.rei"
         pst.pestpp_options["opt_skip_final"] = True
         pst.write(os.path.join(m_d,"freyberg_opt_restart.pst"))
```

```
noptmax:1, npar_adj:26, nnz_obs:4
```

```
In [29]: pyemu.os_utils.run("pestpp-opt freyberg_opt_restart.pst",cwd=m_d)

In [30]: par_df = pyemu.pst_utils.read_parfile(os.path.join(m_d,"freyberg_opt_restart.1.par"))
         print(par_df.loc[dvg_pars,"parval1"].sum())
         par_df.loc[dvg_pars,:]
```

```
13.177556909488672
```

```
Out[30]:                      parnme   parval1  scale  offset
         parnme
         wf0200090016  wf0200090016  3.000000    1.0     0.0
         wf0200110013  wf0200110013  3.000000    1.0     0.0
         wf0200200014  wf0200200014  0.000000    1.0     0.0
         wf0200260010  wf0200260010  1.177557    1.0     0.0
         wf0200290006  wf0200290006  3.000000    1.0     0.0
         wf0200340012  wf0200340012  3.000000    1.0     0.0
```

Oh snap! that means we can do all sort of kewl optimization testing really really fast... we can test a (slightly) risk averse stance too:

```
In [31]: pst.pestpp_options["opt_risk"] = 0.51
         pst.write(os.path.join(m_d,"freyberg_opt_restart.pst"))
         pyemu.os_utils.run("pestpp-opt freyberg_opt_restart.pst",cwd=m_d)
         par_df = pyemu.pst_utils.read_parfile(os.path.join(m_d,"freyberg_opt_restart.1.par"))
         print(par_df.loc[dvg_pars,"parval1"].sum())
         par_df.loc[dvg_pars,:]
```

```
noptmax:1, npar_adj:26, nnz_obs:4
8.857835256056427
```

```
Out[31]:                      parnme   parval1  scale  offset
         parnme
         wf0200090016  wf0200090016  3.000000    1.0     0.0
         wf0200110013  wf0200110013  3.000000    1.0     0.0
         wf0200200014  wf0200200014  2.857835    1.0     0.0
         wf0200260010  wf0200260010  0.000000    1.0     0.0
         wf0200290006  wf0200290006  0.000000    1.0     0.0
         wf0200340012  wf0200340012  0.000000    1.0     0.0
```

Lets use the functionality to evaluate how our OUU problem changes if we use posterior standard deviations - this is a critically important use of the uncertainty analysis from history matching:

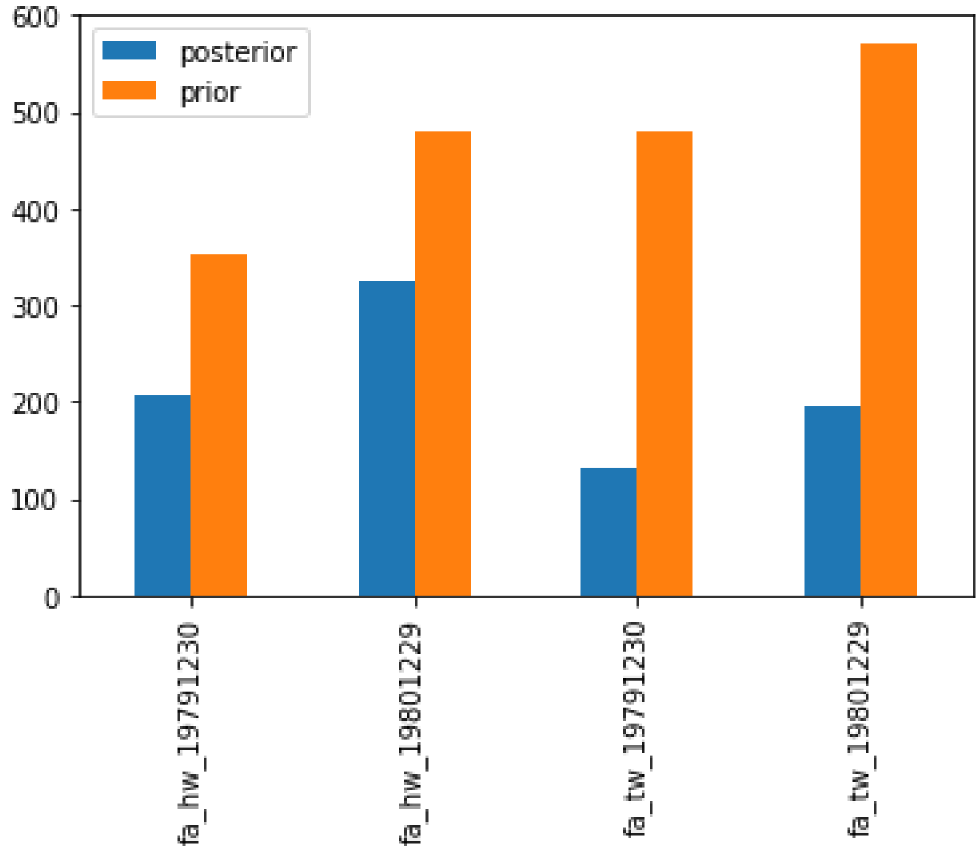
In [32]:
```
obs_df = pd.read_csv(os.path.join("master_ies","freyberg_ies.3.obs.csv"),index_col=0)

#df = df=pd.read_csv(os.path.join("master_glm","freyberg_pp.post.obsen.csv"),index_co
#obs_df = pyemu.ObservationEnsemble.from_dataframe(pst=pst,df=df)
#obs_df = obs_df.loc[obs_df.phi_vector.sort_values().index[:20],:]
pt_std = obs_df.std().loc[pst.nnz_obs_names]
obs_df.std().loc[pst.nnz_obs_names]
#obs_df.max().loc[pst.nnz_obs_names]
```

Out[32]:
```
fa_hw_19791230    207.293769
fa_hw_19801229    324.512508
fa_tw_19791230    130.971667
fa_tw_19801229    195.441533
dtype: float64
```

How much lower is the posterior standard deviations are compared to the prior?

In [33]:
```
pd.DataFrame({"prior":pr_std,"posterior":pt_std}).plot(kind="bar")
```

Out[33]: <matplotlib.axes._subplots.AxesSubplot at 0x181fcea470>



This implies that the chance constraints (which express the important model input uncertainty propogated to the forecast/constraints) is significantly lower, meaning uncertainty has less "value" in the optimization objective function

```
In [34]: pst.observation_data.loc[pst.nnz_obs_names,"weight"] = pt_std.loc[pst.nnz_obs_names]
         pst.observation_data.loc[pst.nnz_obs_names,"weight"]
```

```
Out[34]: obsnme
         fa_hw_19791230    207.293769
         fa_hw_19801229    324.512508
         fa_tw_19791230    130.971667
         fa_tw_19801229    195.441533
         Name: weight, dtype: float64
```

```
In [35]: pst.write(os.path.join(m_d,"freyberg_opt_restart.pst"))
         pyemu.os_utils.run("pestpp-opt freyberg_opt_restart.pst",cwd=m_d)
         par_df = pyemu.pst_utils.read_parfile(os.path.join(m_d,"freyberg_opt_restart.1.par"))
         print(par_df.loc[dvg_pars,"parval1"].sum())
         par_df.loc[dvg_pars,:]
```

```
noptmax:1, npar_adj:26, nnz_obs:4
9.4140209373158
```

```
Out[35]:                     parnme   parval1  scale  offset
         parnme
         wf0200090016  wf0200090016  3.000000    1.0     0.0
         wf0200110013  wf0200110013  3.000000    1.0     0.0
         wf0200200014  wf0200200014  3.000000    1.0     0.0
         wf0200260010  wf0200260010  0.000000    1.0     0.0
         wf0200290006  wf0200290006  0.000000    1.0     0.0
         wf0200340012  wf0200340012  0.414021    1.0     0.0
```

```
In [36]: pyemu.pst_utils.read_resfile(os.path.join(m_d,"freyberg_opt_restart.1.est+fosm.rei"))
```

```
Out[36]:                            name      group  measured    modelled    residual  \
         name
         fa_hw_19791230  fa_hw_19791230  less_than    -300.0 -394.509735   94.509735
         fa_hw_19801229  fa_hw_19801229  less_than    -300.0 -650.145235  350.145235
         fa_tw_19791230  fa_tw_19791230  less_than    -300.0 -433.984934  133.984934
         fa_tw_19801229  fa_tw_19801229  less_than    -300.0 -300.000000    0.000000

                             weight
         name
         fa_hw_19791230  207.293769
         fa_hw_19801229  324.512508
         fa_tw_19791230  130.971667
         fa_tw_19801229  195.441533
```

Again we see that scenarion tail water flux is the binding constraint. So! Lets reformulate the problem to be constrained by the total sw-gw flux across all reaches instead of splitting into headwaters and tailwaters. Good thing we have added the list file budget components to the control file!

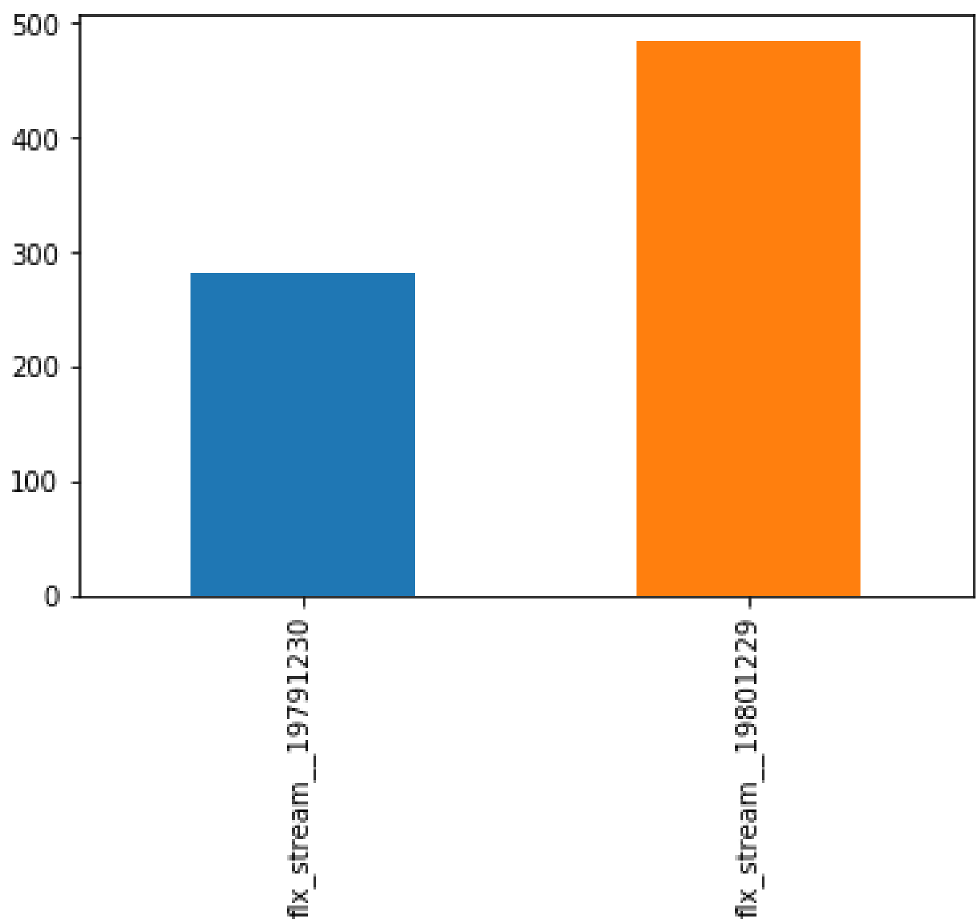
In [37]:
```
pst = pyemu.Pst(os.path.join(m_d,"freyberg_opt_restart.pst"))
obs = pst.observation_data
obs.loc[pst.nnz_obs_names,"obgnme"] = "sw-gw"
obs.loc[pst.nnz_obs_names,"weight"] = 0.0
```

In [38]:
```
tot_swgw = obs.loc[obs.obgnme=="flx_stream_","obsnme"]
```

In [39]:
```
obs.loc[tot_swgw,"obgnme"] = "less_than"
obs.loc[tot_swgw,"weight"] = 1.0
obs.loc[tot_swgw,"weight"] = obs_df.std().loc[pst.nnz_obs_names]
obs.loc[tot_swgw,"obsval"] = -600
```

In [40]:
```
obs_df.std().loc[pst.nnz_obs_names].plot(kind="bar")
```

Out[40]:
```
<matplotlib.axes._subplots.AxesSubplot at 0x181ddb92b0>
```



Since we want to find the most risk averse stance that is still feasible we will run a sweep of risk values:

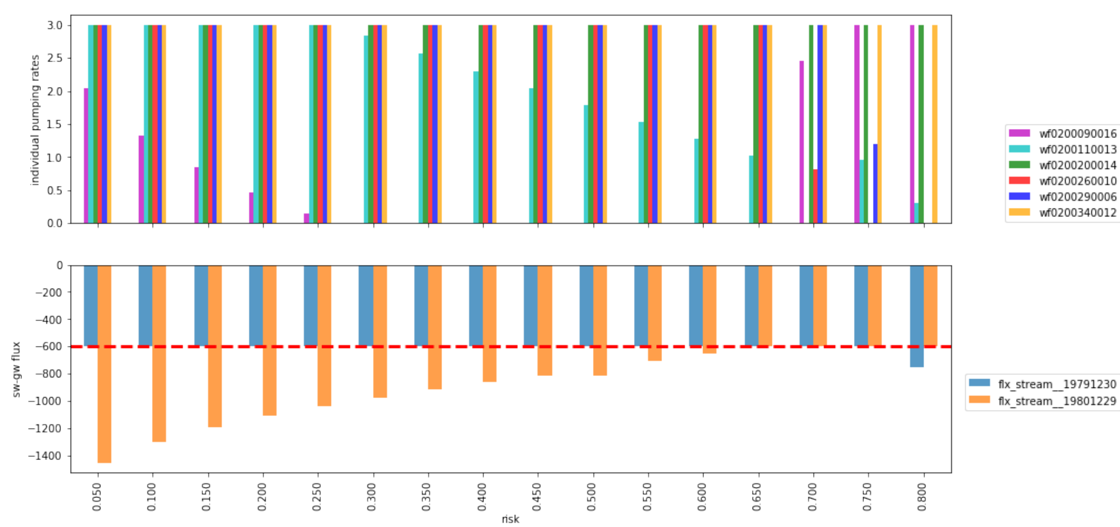
```
In [41]: par_dfs = []
         res_dfs = []
         risk_vals = np.arange(0.05,1.0,0.05)
         for risk in risk_vals:
             #try:
             #    os.remove(os.path.join(m_d,"freyberg_opt_restart.1.est+fosm.rei"))
             #except:
             #    pass

             pst.pestpp_options["opt_risk"] = risk
             pst.pestpp_options["opt_skip_final"] = True
             pst.write(os.path.join(m_d,"freyberg_opt_restart.pst"))
             pyemu.os_utils.run("pestpp-opt freyberg_opt_restart.pst",cwd=m_d)
             par_df = pyemu.pst_utils.read_parfile(os.path.join(m_d,"freyberg_opt_restart.1.pa
             par_df = par_df.loc[dvg_pars,:]
             #when the solution is infeasible, pestpp-opt writes extreme negative values
             # to the par file:
             if par_df.parval1.sum() < 6.0:
                 print("infeasible at risk",risk)
                 break
             res_df = pyemu.pst_utils.read_resfile(os.path.join(m_d,"freyberg_opt_restart.1.es
             res_df = res_df.loc[pst.nnz_obs_names,:]
             res_dfs.append(res_df.modelled)
             par_dfs.append(par_df.parval1)

         # process the dec var and constraint dataframes for plotting
         risk_vals = risk_vals[:len(par_dfs)]
         par_df = pd.concat(par_dfs,axis=1).T
         par_df.index = risk_vals
         par_df.index = par_df.index.map(lambda x: "{0:0.3f}".format(x))
         res_df = pd.concat(res_dfs,axis=1).T
         res_df.index = risk_vals
         res_df.index = res_df.index.map(lambda x: "{0:0.3f}".format(x))
```

```
noptmax:1, npar_adj:26, nnz_obs:2
noptmax:1, npar_adj:26, nnz_obs:2
noptmax:1, npar_adj:26, nnz_obs:2
noptmax:1, npar_adj:26, nnz_obs:2
noptmax:1, npar_adj:26, nnz_obs:2
noptmax:1, npar_adj:26, nnz_obs:2
noptmax:1, npar_adj:26, nnz_obs:2
noptmax:1, npar_adj:26, nnz_obs:2
noptmax:1, npar_adj:26, nnz_obs:2
```

```
noptmax:1, npar_adj:26, nnz_obs:2
noptmax:1, npar_adj:26, nnz_obs:2
noptmax:1, npar_adj:26, nnz_obs:2
noptmax:1, npar_adj:26, nnz_obs:2
noptmax:1, npar_adj:26, nnz_obs:2
noptmax:1, npar_adj:26, nnz_obs:2
noptmax:1, npar_adj:26, nnz_obs:2
noptmax:1, npar_adj:26, nnz_obs:2
infeasible at risk 0.8500000000000001
```

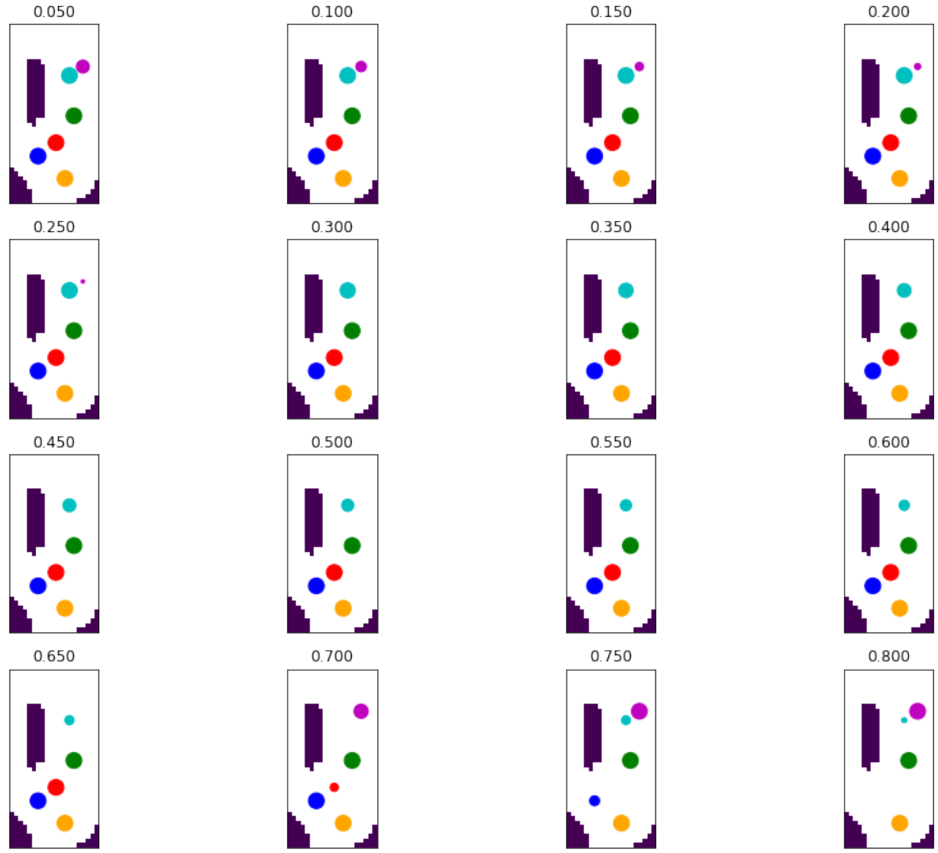
In [42]:
```
colors = ["m","c","g","r","b","orange"]
fig, axes = plt.subplots(2,1,figsize=(15,8))
par_df.plot(kind="bar",ax=axes[0],alpha=0.75,color=colors).legend(bbox_to_anchor=(1.2
axes[0].set_ylabel("individual pumping rates")
axes[0].set_xticklabels([])
res_df.plot(kind="bar",ax=axes[1],alpha=0.75).legend(bbox_to_anchor=(1.2, 0.5))
axes[1].plot(axes[1].get_xlim(),[-600,-600],"r--",lw=3)
axes[1].set_ylabel("sw-gw flux")
axes[1].set_xlabel("risk")
```

Out[42]:
```
Text(0.5, 0, 'risk')
```



In [43]:
```
m = flopy.modflow.Modflow.load("freyberg.nam",model_ws=t_d)
wf_par = pst.parameter_data.loc[dvg_pars,:].copy()
wf_par.loc[:,"k"] = wf_par.parnme.apply(lambda x: int(x[2:4]))
wf_par.loc[:,"i"] = wf_par.parnme.apply(lambda x: int(x[4:8]))
wf_par.loc[:,"j"] = wf_par.parnme.apply(lambda x: int(x[8:]))
wf_par.loc[:,"x"] = wf_par.apply(lambda x: m.sr.xcentergrid[x.i,x.j],axis=1)
wf_par.loc[:,"y"] = wf_par.apply(lambda x: m.sr.ycentergrid[x.i,x.j],axis=1)
```

```python
ib = m.bas6.ibound[0].array
ib = np.ma.masked_where(ib!=0,ib)
fig,axes = plt.subplots(5,int(np.ceil(par_df.shape[0]/5)),figsize=(15,15))
axes = axes.flatten()
for risk,ax in zip(par_df.index,axes):
    ax.set_aspect("equal")
    #ax = plt.subplot(111,aspect="equal")
    ax.imshow(ib,extent=m.sr.get_extent())
    ax.scatter(wf_par.x,wf_par.y,s=par_df.loc[risk,wf_par.parnme].values*50,c=colors)
    ax.set_xticks([])
    ax.set_yticks([])
    ax.set_title(risk)

for i in range(par_df.shape[0],axes.shape[0]):
    ax = axes[i]
    ax.axis("off")
```



how about those figures!!!

How slick was that! no more model runs needed and yet we transformed the OUU problem (by swapping constraints) and solved for a much more risk averse stance! Just to make sure, lets run the model with the most risk-averse decision variables:

```
In [44]: pst.pestpp_options["opt_risk"] = risk_vals[-1]
         pst.pestpp_options["opt_skip_final"] = False
         pst.write(os.path.join(m_d,"freyberg_opt_restart.pst"))
         pyemu.os_utils.run("pestpp-opt freyberg_opt_restart.pst",cwd=m_d)
         # load the simulated outputs plus the FOSM chance constraint offsets:
         res_df = pyemu.pst_utils.read_resfile(os.path.join(m_d,"freyberg_opt_restart.1.sim+fo
         res_df = res_df.loc[pst.nnz_obs_names,:]
         res_df
```

```
noptmax:1, npar_adj:26, nnz_obs:2
```

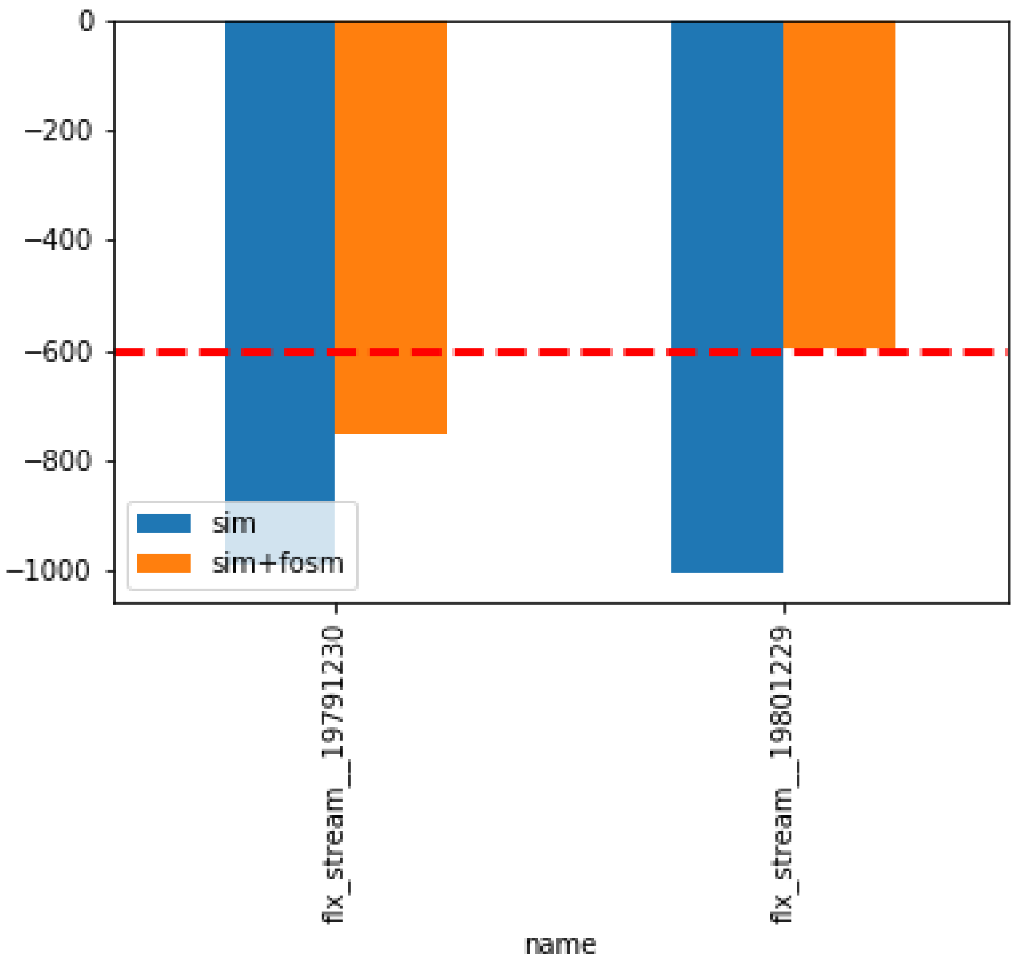
Out[44]:

```
                                          name      group  measured    modelled  \
name
flx_stream__19791230  flx_stream__19791230  less_than    -600.0 -751.541317
flx_stream__19801229  flx_stream__19801229  less_than    -600.0 -599.684272

                        residual      weight
name
flx_stream__19791230  151.541317  282.331881
flx_stream__19801229   -0.315728  483.362732
```

In [45]:

```
# load the actual model simulated outputs
res_df_sim = pyemu.pst_utils.read_resfile(os.path.join(m_d,"freyberg_opt_restart.1.sim
res_df_sim = res_df_sim.loc[pst.nnz_obs_names,:]
ax = pd.DataFrame({"sim":res_df_sim.modelled,"sim+fosm":res_df.modelled}).plot(kind="l
ax.plot(ax.get_xlim(),[-600,-600],"r--",lw=3)
```

Out[45]: [<matplotlib.lines.Line2D at 0x181eb99fd0>]



Here we can see the cost of uncertainty - we have to simulate a greater flux from gw to sw to make sure (e.g. be risk averse) that the flux from gw to sw is actually at least 600 m3/day

2 FINALLY!!!

We now see the reason for high-dimensional uncertainty quantification and history matching: to define and then reduce (through data assimulation) the uncertainty in the model-based constraints (e.g. sw-gw forecasts) so that we can find a more risk-averse management solution - we can use to model to identify an optimal pumping scheme to provide the volume of water needed for supply/ag but also provide assurances (at the given confidence) that ecological flows will be maintained under both current conditions and in the event of an extreme 1-year drought. BOOM!