pestpp-opt

July 19, 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]:
```
%matplotlib inline
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
%matplotlib inline
```

```
flopy is installed in C:\Users\knowling\Dev\GW1876\activities_csiro\notebooks\flopy
```

1.1 SUPER IMPORTANT: SET HOW MANY PARALLEL WORKERS TO USE

In [2]:
```
num_workers = 20
```

In [3]:
```
t_d = "template"
m_d = "master_opt"
```

1.1.1 We can look at the summary information about the parameters

In [4]:
```
pst = pyemu.Pst(os.path.join(t_d,"freyberg.pst"))
pst.write_par_summary_table(filename="none").sort_index()
```

Out[4]:
```
                    type transform  count  initial value  upper bound  \
cn_hk6             cn_hk6       log      1              0            1
cn_hk7             cn_hk7       log      1              0            1
cn_hk8             cn_hk8       log      1              0            1
cn_prsity6    cn_prsity6       log      1              0    0.0791812
cn_prsity7    cn_prsity7       log      1              0    0.0791812
```

cn_prsity8	cn_prsity8	log	1	0	0.0791812
cn_rech4	cn_rech4	log	1	0	0.0413927
cn_rech5	cn_rech5	log	1	0	0.0413927
cn_ss6	cn_ss6	log	1	0	1
cn_ss7	cn_ss7	log	1	0	1
cn_ss8	cn_ss8	log	1	0	1
cn_strt6	cn_strt6	log	1	0	0.0211893
cn_strt7	cn_strt7	log	1	0	0.0211893
cn_strt8	cn_strt8	log	1	0	0.0211893
cn_sy6	cn_sy6	log	1	0	0.243038
cn_sy7	cn_sy7	log	1	0	0.243038
cn_sy8	cn_sy8	log	1	0	0.243038
cn_vka6	cn_vka6	log	1	0	1
cn_vka7	cn_vka7	log	1	0	1
cn_vka8	cn_vka8	log	1	0	1
drncond_k00	drncond_k00	log	10	0	1
flow	flow	log	1	0	0.09691
gr_hk3	gr_hk3	log	705	0	1
gr_hk4	gr_hk4	log	705	0	1
gr_hk5	gr_hk5	log	705	0	1
gr_prsity3	gr_prsity3	log	705	0	0.0791812
gr_prsity4	gr_prsity4	log	705	0	0.0791812
gr_prsity5	gr_prsity5	log	705	0	0.0791812
gr_rech2	gr_rech2	log	705	0	0.0413927
gr_rech3	gr_rech3	log	705	0	0.0413927
...	...	...	...	...	...
gr_strt5	gr_strt5	log	705	0	0.0211893
gr_sy3	gr_sy3	log	705	0	0.243038
gr_sy4	gr_sy4	log	705	0	0.243038
gr_sy5	gr_sy5	log	705	0	0.243038
gr_vka3	gr_vka3	log	705	0	1
gr_vka4	gr_vka4	log	705	0	1
gr_vka5	gr_vka5	log	705	0	1
pp_hk0	pp_hk0	log	32	0	1
pp_hk1	pp_hk1	log	32	0	1
pp_hk2	pp_hk2	log	32	0	1
pp_prsity0	pp_prsity0	log	32	0	0.0791812
pp_prsity1	pp_prsity1	log	32	0	0.0791812
pp_prsity2	pp_prsity2	log	32	0	0.0791812
pp_rech0	pp_rech0	log	32	0	0.0413927
pp_rech1	pp_rech1	log	32	0	0.0413927
pp_ss0	pp_ss0	log	32	0	1
pp_ss1	pp_ss1	log	32	0	1
pp_ss2	pp_ss2	log	32	0	1
pp_strt0	pp_strt0	log	32	0	0.0211893
pp_strt1	pp_strt1	log	32	0	0.0211893
pp_strt2	pp_strt2	log	32	0	0.0211893
pp_sy0	pp_sy0	log	32	0	0.243038

pp_sy1	pp_sy1	log	32	0	0.243038
pp_sy2	pp_sy2	log	32	0	0.243038
pp_vka0	pp_vka0	log	32	0	1
pp_vka1	pp_vka1	log	32	0	1
pp_vka2	pp_vka2	log	32	0	1
strk	strk	log	40	0	2
welflux	welflux	log	2	0	1
welflux_k02	welflux_k02	log	6	0	1

	lower bound	standard deviation
cn_hk6	-1	0.5
cn_hk7	-1	0.5
cn_hk8	-1	0.5
cn_prsity6	-0.09691	0.0440228
cn_prsity7	-0.09691	0.0440228
cn_prsity8	-0.09691	0.0440228
cn_rech4	-0.0457575	0.0217875
cn_rech5	-0.0457575	0.0217875
cn_ss6	-1	0.5
cn_ss7	-1	0.5
cn_ss8	-1	0.5
cn_strt6	-0.0222764	0.0108664
cn_strt7	-0.0222764	0.0108664
cn_strt8	-0.0222764	0.0108664
cn_sy6	-0.60206	0.211275
cn_sy7	-0.60206	0.211275
cn_sy8	-0.60206	0.211275
cn_vka6	-1	0.5
cn_vka7	-1	0.5
cn_vka8	-1	0.5
drncond_k00	-1	0.5
flow	-0.124939	0.0554622
gr_hk3	-1	0.5
gr_hk4	-1	0.5
gr_hk5	-1	0.5
gr_prsity3	-0.09691	0.0440228
gr_prsity4	-0.09691	0.0440228
gr_prsity5	-0.09691	0.0440228
gr_rech2	-0.0457575	0.0217875
gr_rech3	-0.0457575	0.0217875
...	...	...
gr_strt5	-0.0222764	0.0108664
gr_sy3	-0.60206	0.211275
gr_sy4	-0.60206	0.211275
gr_sy5	-0.60206	0.211275
gr_vka3	-1	0.5
gr_vka4	-1	0.5
gr_vka5	-1	0.5

```
pp_hk0              -1             0.5
pp_hk1              -1             0.5
pp_hk2              -1             0.5
pp_prsity0    -0.09691       0.0440228
pp_prsity1    -0.09691       0.0440228
pp_prsity2    -0.09691       0.0440228
pp_rech0    -0.0457575       0.0217875
pp_rech1    -0.0457575       0.0217875
pp_ss0              -1             0.5
pp_ss1              -1             0.5
pp_ss2              -1             0.5
pp_strt0    -0.0222764       0.0108664
pp_strt1    -0.0222764       0.0108664
pp_strt2    -0.0222764       0.0108664
pp_sy0        -0.60206        0.211275
pp_sy1        -0.60206        0.211275
pp_sy2        -0.60206        0.211275
pp_vka0             -1             0.5
pp_vka1             -1             0.5
pp_vka2             -1             0.5
strk                -2               1
welflux             -1             0.5
welflux_k02         -1             0.5

[65 rows x 7 columns]
```

1.1.2 define our decision variable 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!

Define a parameter group as the devision variables (i.e. the variables that we will tune to meet the optimal condition). We will define `wellflux_k02` as the decision variable group (defined by the `++arg` called `opt_dec_var_groups`. Note in the table above that this group represents (time-invariant) flux mulipliers for each of the 6 wells (we will however only optimize for pumping rates in current (historic) conditions).

We can also define which direction we want the optimization to go using `opt_direction` as `max`. This means the objective of the optimization will be to maximize future pumping subject to the constraints we will establish below.

```
In [5]: pst.pestpp_options = {}
        #dvg = ["welflux_k02","welflux"]
        dvg = ["welflux_k02"]  # time-invariant flux multiplier for each well
        pst.pestpp_options["opt_dec_var_groups"] = dvg
        pst.pestpp_options["opt_direction"] = "max"
```

For the first run, we won't use chance constraints, so just fix all non-decision-variable "parameters". 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. For typical parameter estimation, `derinc=0.01` is often sufficient for calculating a Jacobian matrix. But, for the response matrix method of optimization, the response can be subtle requiring a greater perturbation increment. We will set it to `0.25` using some `pandas` manipulation.

In [6]:
```
par = pst.parameter_data
par.loc[:,"partrans"] = "fixed"

#  first turn off pumping rate in the scenario stress period (mask dec vars)
par.loc["welflux_001","parlbnd"] = 0.0
par.loc["welflux_001","parval1"] = 0.0

# dec vars
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  # corresponds to -450 m3/d
par.loc[dvg_pars,"parval1"] = 1.0

par.loc[dvg_pars,:]
```

Out[6]:
```
                   parnme partrans parchglim  parval1  parlbnd  parubnd  \
parnme
wf0200090016  wf0200090016     none    factor      1.0      0.0      3.0
wf0200110013  wf0200110013     none    factor      1.0      0.0      3.0
wf0200200014  wf0200200014     none    factor      1.0      0.0      3.0
wf0200260010  wf0200260010     none    factor      1.0      0.0      3.0
wf0200290006  wf0200290006     none    factor      1.0      0.0      3.0
wf0200340012  wf0200340012     none    factor      1.0      0.0      3.0

                    pargp  scale  offset  dercom  extra
parnme
wf0200090016  welflux_k02    1.0     0.0       1    NaN
wf0200110013  welflux_k02    1.0     0.0       1    NaN
wf0200200014  welflux_k02    1.0     0.0       1    NaN
wf0200260010  welflux_k02    1.0     0.0       1    NaN
wf0200290006  welflux_k02    1.0     0.0       1    NaN
wf0200340012  welflux_k02    1.0     0.0       1    NaN
```

In [7]:
```
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[7]:
```
                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
```

1.1.3 define constraints

Model-based or dec var-related constraints are identified in pestpp-opt by an obs or prior information 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 [8]:
```
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[8]:
```
                            obsnme     obsval  weight obgnme  extra
obsnme
fa_hw_19791230  fa_hw_19791230 -991.84964     0.0  flaqx    NaN
fa_hw_19801229  fa_hw_19801229 -941.75610     0.0  flaqx    NaN
fa_tw_19791230  fa_tw_19791230 -747.40120     0.0  flaqx    NaN
fa_tw_19801229  fa_tw_19801229 -669.89580     0.0  flaqx    NaN
```

We need to change the obs group (obgnme) so that pestpp-opt will recognize these model outputs as constraints. The obsval becomes the RHS of the constraint.

In [9]:
```
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
```

In [10]:
```
# We can also set a lower bound constraint on the total abstraction rate
#(good thing we included all those list file budget components as observations!)

# 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 variable values - the required minimum value will the sum of current pumping rates:

In [11]:
```
pyemu.pst_utils.pst_config["prior_fieldnames"]
```

```
Out[11]: ['pilbl', 'equation', 'weight', 'obgnme']
```

Since all pumping wells are using the same rate and are of same "water supply benefit", 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 [12]: 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[12]: '1.0 * wf0200090016 + 1.0 * wf0200110013 + 1.0 * wf0200200014 + 1.0 * wf0200260010 + 1
```

```
In [13]: pst.prior_information
```

```
Out[13]:             obgnme pilbl  \
         pi_1  greater_than  pi_1


         pi_1  1.0 * wf0200090016 + 1.0 * wf0200110013 + 1.0 * wf0200200014 + 1.0 * wf02002600

               weight
         pi_1     1.0
```

1.2 now for a risk-neutral optimization (ignoring uncertainty in constraints)

Note that setting `noptmax=1` is equivalent to selecting Linear Programming (LP) as the optimization algorithm (thus assuming a linear response matrix).

A higher value of `noptmax` runs Sequential Linear Programming (SLP)

```
In [14]: 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=num_workers
```

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

Let's load and inspect the response matrix

```
In [15]: jco = pyemu.Jco.from_binary(os.path.join(m_d,"freyberg_opt.1.jcb")).to_dataframe().loc
         jco
```

```
Out[15]:                 wf0200090016  wf0200110013  wf0200200014  wf0200260010  \
         fa_hw_19791230     137.57200     126.32400      46.30000       21.9080
         fa_hw_19801229      22.66400      28.77600      12.08000       12.3920
         fa_tw_19791230       6.50728      14.53516      93.28136       92.4232
```

```
fa_tw_19801229       4.11600       7.64240      15.33680       31.0356

                 wf0200290006  wf0200340012
fa_hw_19791230       18.12000        4.8320
fa_hw_19801229       13.28800        3.4040
fa_tw_19791230       71.84608       82.9612
fa_tw_19801229       35.01240       17.5824
```

We see the transient effects in the nonzero value between current pumping rates (columns) and scenario sw-gw exchange (rows from 1980) and that the current 1979 sw-gw exchanges are always larger than those in the scenario 1980 condition.

Let's also load the optimal decision variable values:

```
In [16]: 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,:]
```

```
11.843760938848522
```

```
Out[16]:                     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  0.000000    1.0     0.0
         wf0200290006  wf0200290006  3.000000    1.0     0.0
         wf0200340012  wf0200340012  2.843761    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 [17]: 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[17]:                           name      group  measured   modelled   residual  \
         name
         fa_hw_19791230  fa_hw_19791230  less_than    -300.0 -472.60565  172.60565
         fa_hw_19801229  fa_hw_19801229  less_than    -300.0 -931.20600  631.20600
         fa_tw_19791230  fa_tw_19791230  less_than    -300.0 -299.65330   -0.34670
         fa_tw_19801229  fa_tw_19801229  less_than    -300.0 -454.61650  154.61650

                         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 (or "active") constraint is the one closest to its RHS

We better also check that our prior information constraint (min total abstracted water allocation) is being met..

```
In [18]: pst.res.loc[pst.prior_names,:]
```

```
Out[18]:       name         group  measured  modelled  residual  weight
         name
         pi_1  pi_1  greater_than       6.0       6.0       0.0     1.0
```

1.2.1 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 specify 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 [19]: 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 [20]: cn_pars = par.loc[par.pargp.apply(lambda x: "cn" in x),"parnme"]
         cn_pars
```

```
Out[20]: 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 [21]:
```
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). Given that we only have 6 decision variables, let's just re-populate the response matrix while also populating the Jacobian.

In [22]:
```
pyemu.os_utils.start_slaves(t_d,"pestpp-opt","freyberg_opt_uu1.pst",num_slaves=num_wo
```

What do we expect to see here? What should happen to the optimal dec vars? And the constraints?

In [23]:
```
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[23]:

name	name	group	measured	modelled	residual
fa_hw_19791230	fa_hw_19791230	less_than	-300.0	-457.77507	157.77507
fa_hw_19801229	fa_hw_19801229	less_than	-300.0	-922.64900	622.64900
fa_tw_19791230	fa_tw_19791230	less_than	-300.0	-226.97920	-73.02080
fa_tw_19801229	fa_tw_19801229	less_than	-300.0	-431.59970	131.59970

name	weight
fa_hw_19791230	1.0
fa_hw_19801229	1.0
fa_tw_19791230	1.0
fa_tw_19801229	1.0

In [24]:
```
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,:]
```

```
12.645484225593641
```

Out[24]:

parnme	parnme	parval1	scale	offset
wf0200090016	wf0200090016	3.000000	1.0	0.0

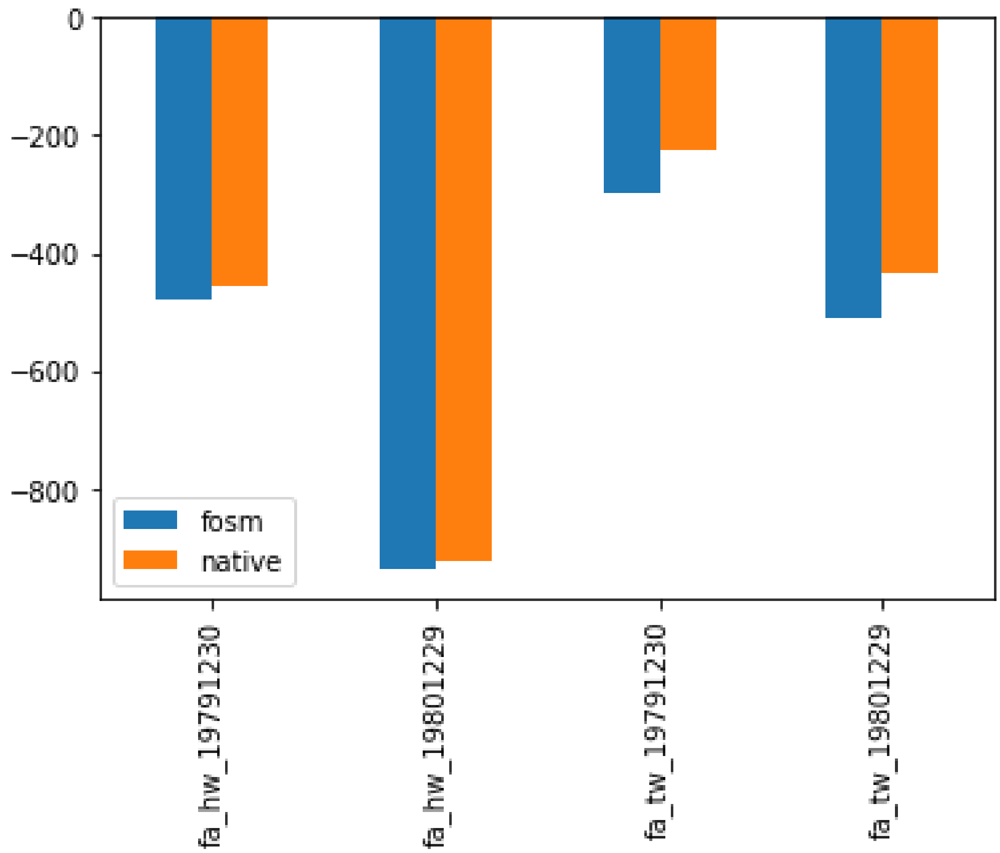
```
wf0200110013  wf0200110013  3.000000    1.0     0.0
wf0200200014  wf0200200014  0.000000    1.0     0.0
wf0200260010  wf0200260010  0.645484    1.0     0.0
wf0200290006  wf0200290006  3.000000    1.0     0.0
wf0200340012  wf0200340012  3.000000    1.0     0.0
```

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 [25]:
```
res_df = pyemu.pst_utils.read_resfile(os.path.join(m_d,"freyberg_opt_uu1.1.sim+fosm.re
res_df
```

Out[25]:
```
                            name      group  measured    modelled    residual  \
name
fa_hw_19791230  fa_hw_19791230  less_than    -300.0 -478.132661  178.132661
fa_hw_19801229  fa_hw_19801229  less_than    -300.0 -939.192585  639.192585
fa_tw_19791230  fa_tw_19791230  less_than    -300.0 -299.598698   -0.401302
fa_tw_19801229  fa_tw_19801229  less_than    -300.0 -508.738046  208.738046

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

In [26]:
```
ax = pd.DataFrame({"native":pst.res.modelled,"fosm":res_df.modelled}).loc[pst.nnz_obs_
plt.show()
```



1.2.2 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 (i.e. uncertainty in the forecasts/constraints). These can be derived from our existing ensembles (oh snap!)

In [27]:
```
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 [28]:
```
pr_std = obs_df.std().loc[pst.nnz_obs_names]
pr_std
```

Out[28]:
```
fa_hw_19791230     598.866581
fa_hw_19801229     986.548558
fa_tw_19791230     729.480402
fa_tw_19801229    1049.379733
dtype: float64
```

Note we can also skip the FOSM calcs within `PESTPP-OPT` using weights as per previous FOSM standard deviation calcs, not just ensemble-based standard deviations

```
In [29]: 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 [30]: pyemu.os_utils.start_slaves(t_d,"pestpp-opt","freyberg_opt_uu2.pst",num_slaves=num_wo
```

```
In [31]: 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,:]
```

```
13.859431873570639
```

Out[31]:

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	1.859432	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 that we used for the FOSM calcs within PESTPP-OPT?

1.2.3 Super secret mode for `LP`

It 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!?

As long as the same decision variables are relates to the same responses, and we can fairly assume that the response matrix that relates the decision variables to the constraints is linear, then the response matrix doesn't change even if things like bounds and risk level change. We just need `pestpp-opt` to read in the response matrix (which is stored with the same format as a Jacobian (`jcb`)) and the residuals (`rei`).

This is done by specifying some additional ++args (and copying some files around)

```
In [32]: 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
```

```
Out[32]: 'master_opt\\restart.rei'
```

Once we have copied over the necessary files, we set a few ++args:
* `base_jacobian`: this instructs `pestpp-opt` to read in the existing response matrix *

hotstart_resfile: this instructs pestpp-opt to use the residuals we already have * opt_skip_final: this waives the usual practice of running the model once with optimal parameter values

Which runs do each of these skip specifically?

```
In [33]: 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 [34]: pyemu.os_utils.run("pestpp-opt freyberg_opt_restart.pst",cwd=m_d)
```

```
In [35]: 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,:]
```

```
13.859431873570639
```

Out[35]:

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	1.859432	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...

1.3 now let's try taking a risk averse stance

```
In [36]: risk = 0.55
```

```
In [37]: pst.pestpp_options["opt_risk"] = risk
         pst.write(os.path.join(m_d,"freyberg_opt_restart.pst"))
         pyemu.os_utils.run("pestpp-opt freyberg_opt_restart.pst",cwd=m_d)
```

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

```
In [38]: 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,:]
```

```
10.738811001362457
```

Out[38]:

	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	0.000000	1.0	0.0
wf0200290006	wf0200290006	3.000000	1.0	0.0
wf0200340012	wf0200340012	1.738811	1.0	0.0

1.3.1 now lets 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...

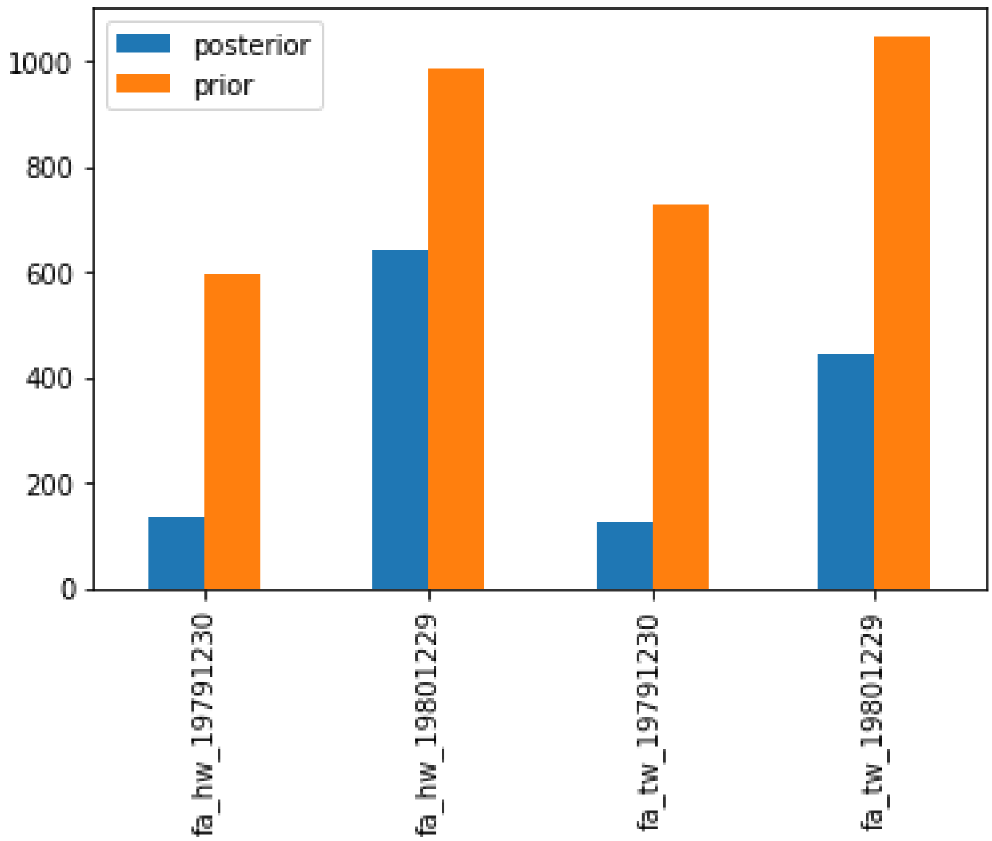
In [39]:
```
obs_df = pd.read_csv(os.path.join("master_ies","freyberg_ies.3.obs.csv"),index_col=0)

#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[39]:
```
fa_hw_19791230    137.209527
fa_hw_19801229    644.750474
fa_tw_19791230    126.348657
fa_tw_19801229    447.159160
dtype: float64
```

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

In [40]:
```
pd.DataFrame({"prior":pr_std,"posterior":pt_std}).plot(kind="bar")
```

Out[40]:
```
<matplotlib.axes._subplots.AxesSubplot at 0x1d4ebf71080>
```



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 [41]: 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[41]: obsnme
         fa_hw_19791230    137.209527
         fa_hw_19801229    644.750474
         fa_tw_19791230    126.348657
         fa_tw_19801229    447.159160
         Name: weight, dtype: float64
```

```
In [42]: pst.write(os.path.join(m_d,"freyberg_opt_restart.pst"))
         pyemu.os_utils.run("pestpp-opt freyberg_opt_restart.pst",cwd=m_d)
```

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

```
In [43]: 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,:]
```

```
11.652379593698083
```

Out[43]:

```
                          parnme   parval1  scale  offset
parnme
wf0200090016  wf0200090016  3.00000    1.0     0.0
wf0200110013  wf0200110013  3.00000    1.0     0.0
wf0200200014  wf0200200014  0.00000    1.0     0.0
wf0200260010  wf0200260010  0.00000    1.0     0.0
wf0200290006  wf0200290006  3.00000    1.0     0.0
wf0200340012  wf0200340012  2.65238    1.0     0.0
```

In [44]:

```
pyemu.pst_utils.read_resfile(os.path.join(m_d,"freyberg_opt_restart.1.est+fosm.rei"))
```

Out[44]:

```
                          name      group  measured    modelled    residual  \
name
fa_hw_19791230  fa_hw_19791230  less_than    -300.0 -456.188677  156.188677
fa_hw_19801229  fa_hw_19801229  less_than    -300.0 -851.274660  551.274660
fa_tw_19791230  fa_tw_19791230  less_than    -300.0 -300.000000    0.000000
fa_tw_19801229  fa_tw_19801229  less_than    -300.0 -402.224583  102.224583

                    weight
name
fa_hw_19791230  137.209527
fa_hw_19801229  644.750474
fa_tw_19791230  126.348657
fa_tw_19801229  447.159159
```

Again we see that historic tail water flux is the binding constraint.

1.4 some reformulation of the opt problem. Can we open up decision variable (feasibility) space?

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 [45]:

```
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"  # hw and tw constraints from tagged "l
obs.loc[pst.nnz_obs_names,"weight"] = 0.0
```

In [46]:

```
tot_swgw = obs.loc[obs.obgnme.str.startswith("flx_stream_"),"obsnme"]
tot_swgw
```

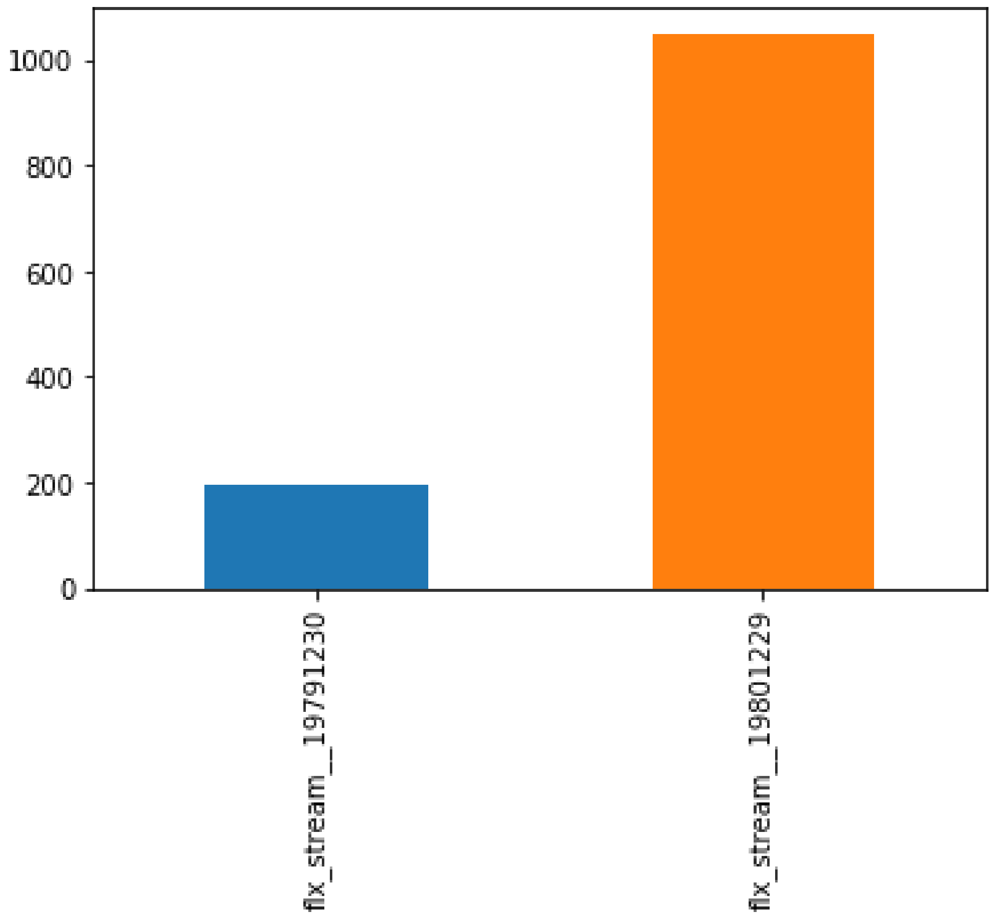
Out[46]:

```
obsnme
flx_stream__19791230    flx_stream__19791230
flx_stream__19801229    flx_stream__19801229
Name: obsnme, dtype: object
```

```
In [47]: 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  # simple linear sum
```

```
In [48]: obs_df.std().loc[pst.nnz_obs_names].plot(kind="bar")
```

```
Out[48]: <matplotlib.axes._subplots.AxesSubplot at 0x1d4ebf32240>
```



1.5 risk sweeps

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

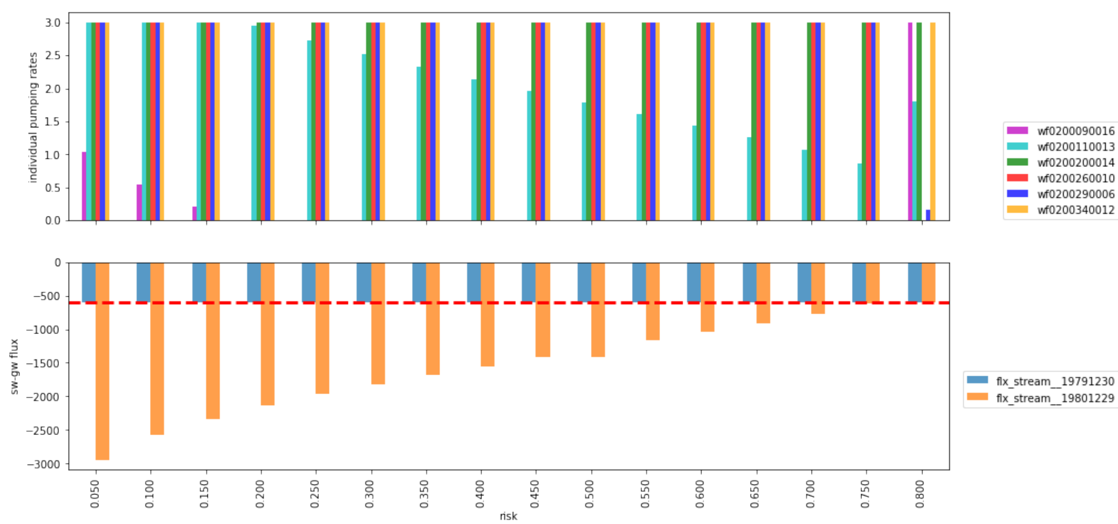
```
In [49]: par_dfs = []
         res_dfs = []
         risk_vals = np.arange(0.05,1.0,0.05)
         for risk in risk_vals:
```

```
            #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
            print("undertaking evaluation for risk value: {0:.2f}".format(risk))
            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 {0:.2f}".format(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))
```

```
undertaking evaluation for risk value: 0.05
noptmax:1, npar_adj:26, nnz_obs:2
undertaking evaluation for risk value: 0.10
noptmax:1, npar_adj:26, nnz_obs:2
undertaking evaluation for risk value: 0.15
noptmax:1, npar_adj:26, nnz_obs:2
undertaking evaluation for risk value: 0.20
noptmax:1, npar_adj:26, nnz_obs:2
undertaking evaluation for risk value: 0.25
noptmax:1, npar_adj:26, nnz_obs:2
undertaking evaluation for risk value: 0.30
noptmax:1, npar_adj:26, nnz_obs:2
undertaking evaluation for risk value: 0.35
noptmax:1, npar_adj:26, nnz_obs:2
undertaking evaluation for risk value: 0.40
```

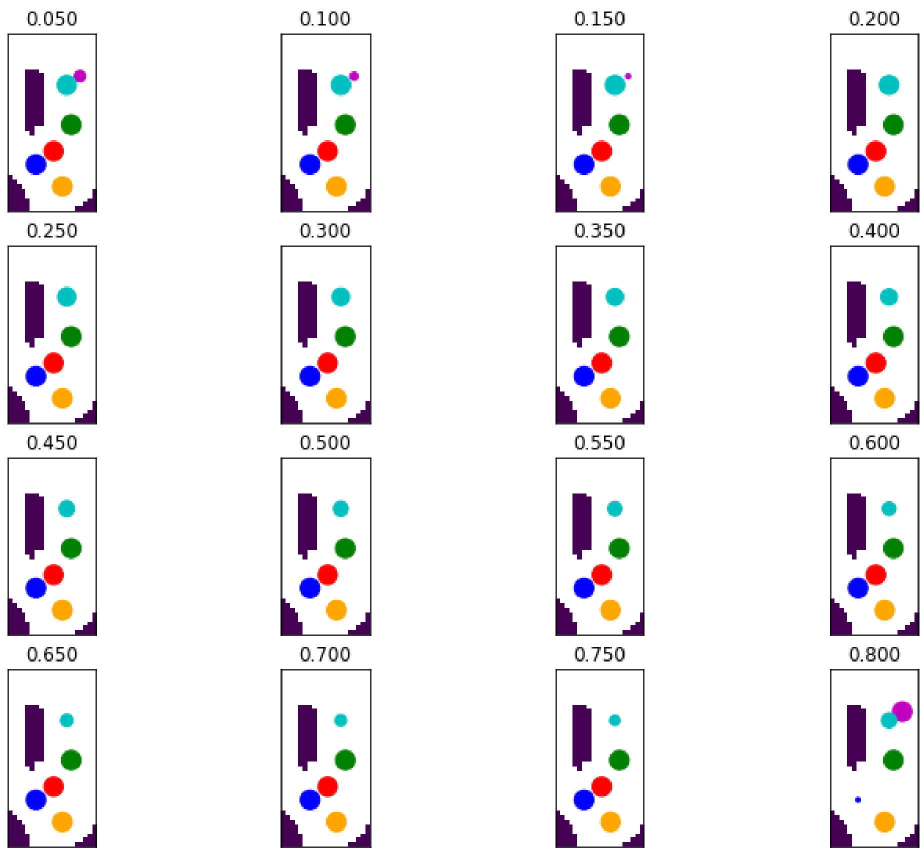
```
noptmax:1, npar_adj:26, nnz_obs:2
undertaking evaluation for risk value: 0.45
noptmax:1, npar_adj:26, nnz_obs:2
undertaking evaluation for risk value: 0.50
noptmax:1, npar_adj:26, nnz_obs:2
undertaking evaluation for risk value: 0.55
noptmax:1, npar_adj:26, nnz_obs:2
undertaking evaluation for risk value: 0.60
noptmax:1, npar_adj:26, nnz_obs:2
undertaking evaluation for risk value: 0.65
noptmax:1, npar_adj:26, nnz_obs:2
undertaking evaluation for risk value: 0.70
noptmax:1, npar_adj:26, nnz_obs:2
undertaking evaluation for risk value: 0.75
noptmax:1, npar_adj:26, nnz_obs:2
undertaking evaluation for risk value: 0.80
noptmax:1, npar_adj:26, nnz_obs:2
undertaking evaluation for risk value: 0.85
noptmax:1, npar_adj:26, nnz_obs:2
infeasible at risk 0.85
```

In [50]:
```
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");
```



Now for some maps of pumping regimes

In [51]:
```
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)

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=(12,12))
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 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:

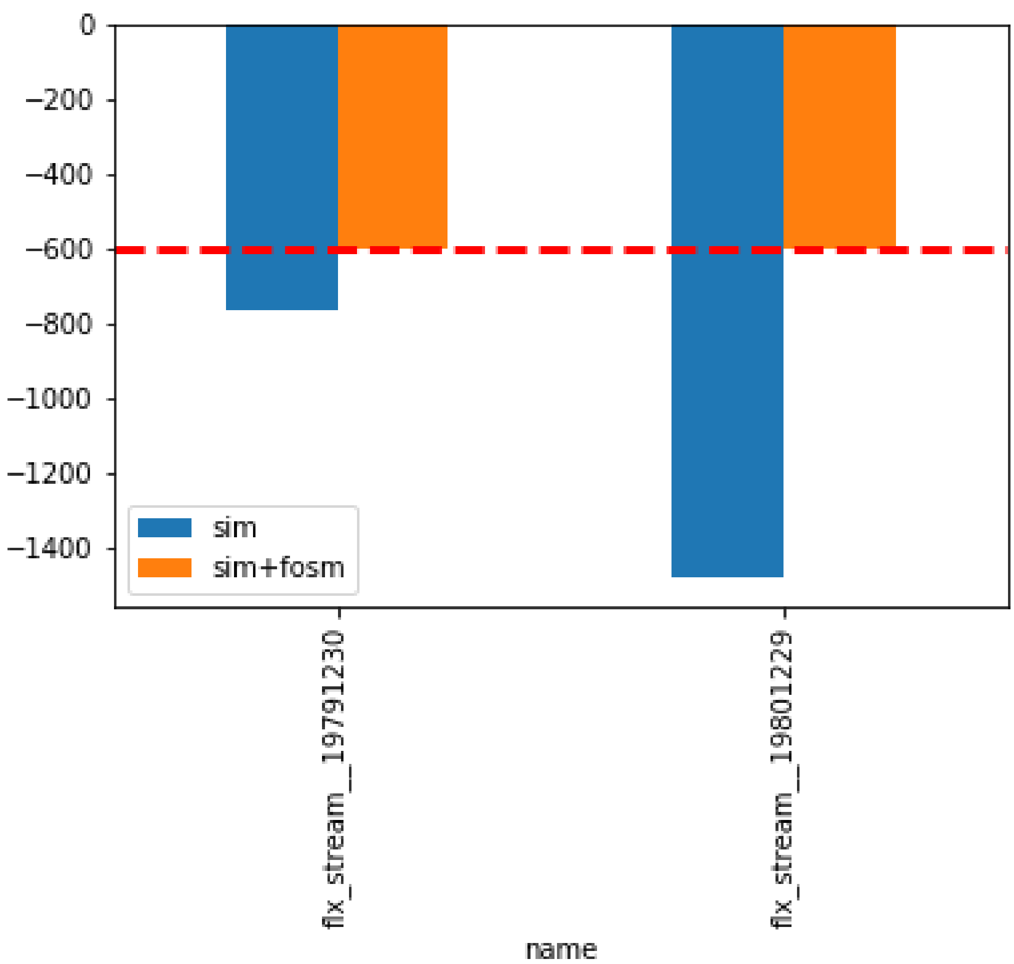
```
In [52]: pst.pestpp_options["opt_risk"] = risk_vals[-1]
         pst.pestpp_options["opt_skip_final"] = False
         pst.write(os.path.join(m_d,"freyberg_opt_restart.pst"))
         pyemu.os_utils.run("pestpp-opt freyberg_opt_restart.pst",cwd=m_d)
         # load the simulated outputs plus the FOSM chance constraint offsets:
         res_df = pyemu.pst_utils.read_resfile(os.path.join(m_d,"freyberg_opt_restart.1.sim+fos
         res_df = res_df.loc[pst.nnz_obs_names,:]
         res_df
```

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

Out[52]:
```
                                       name      group  measured    modelled  \
name
flx_stream__19791230  flx_stream__19791230  less_than    -600.0 -599.913176
flx_stream__19801229  flx_stream__19801229  less_than    -600.0 -599.505308

                      residual       weight
name
flx_stream__19791230 -0.086824   194.650950
flx_stream__19801229 -0.494692  1047.595606
```

In [53]:
```
# 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="
ax.plot(ax.get_xlim(),[-600,-600],"r--",lw=3)
```

Out[53]: [<matplotlib.lines.Line2D at 0x1d4ec814160>]



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 assimilation) 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 a model to identify an optimal pumping scheme to provide the volume of water needed for water supply, agriculture, etc. 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!