pestpp-opt

May 31, 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
```

1.1 SUPER IMPORTANT: SET HOW MANY PARALLEL WORKERS TO USE

```
In [2]: num_workers = 10
```

```
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  \
        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]
```

1.1.2 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!

Define a parameter group as the devision variables (e.g. 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 this represents 6 wells in the future.

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"]
        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 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. 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.

4

```
In [6]: 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[6]:

	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 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 [7]: 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[7]:

	obsnme	obsval	weight	obgnme	extra
obsnme					
fa_hw_19791230	fa_hw_19791230	-718.89590	0.0	flaqx	NaN
fa_hw_19801229	fa_hw_19801229	348.94346	0.0	flaqx	NaN
fa_tw_19791230	fa_tw_19791230	-38.23214	0.0	flaqx	NaN
fa_tw_19801229	fa_tw_19801229	789.05020	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 [8]: 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 [9]: pyemu.pst_utils.pst_config["prior_fieldnames"]

Out[9]: ['pilbl', 'equation', 'weight', 'obgnme']
```

Since all pumping wells 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 [10]: 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[10]: '1.0 * wf0200090016 + 1.0 * wf0200110013 + 1.0 * wf0200200014 + 1.0 * wf0200260010 +

In [11]: pst.prior_information

Out[11]:              obgnme pilbl  \
         pi_1  greater_than  pi_1


         pi_1  1.0 * wf0200090016 + 1.0 * wf0200110013 + 1.0 * wf0200200014 + 1.0 * wf0200260001


                  weight
         pi_1     1.0
```

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

6

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

```
In [12]: 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_worker
```

noptmax:1, npar_adj:6, nnz_obs:4

Let's load and inspect the response matrix

```
In [13]: jco = pyemu.Jco.from_binary(os.path.join(m_d,"freyberg_opt.1.jcb")).to_dataframe().lo
         jco
```

```
Out[13]:                     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 [14]: 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[14]:                   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 [15]: 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[15]:                             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

1.1.4   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 [16]: pst.pestpp_options["opt_risk"] = 0.4
```

For the FOSM-based chance constraints, we also need to have at least one adjustable non-decvar 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 [17]: cn_pars = par.loc[par.pargp.apply(lambda x: "cn" in x),"parnme"]
         cn_pars

Out[17]: 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 [18]: 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 [19]: pyemu.os_utils.start_slaves(t_d,"pestpp-opt","freyberg_opt_uu1.pst",num_slaves=num_wor
```

```
In [20]: 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[20]:                         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 [21]: m_d
```

```
Out[21]: 'master_opt'
```

```
In [22]: 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[22]:                            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 [23]: res_df = pyemu.pst_utils.read_resfile(os.path.join(m_d,"freyberg_opt_uu1.1.sim+fosm.re
         res_df
```

```
Out[23]:                            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 [24]: ax = pd.DataFrame({"native":pst.res.modelled,"fosm":res_df.modelled}).loc[pst.nnz_obs
         plt.show()
```
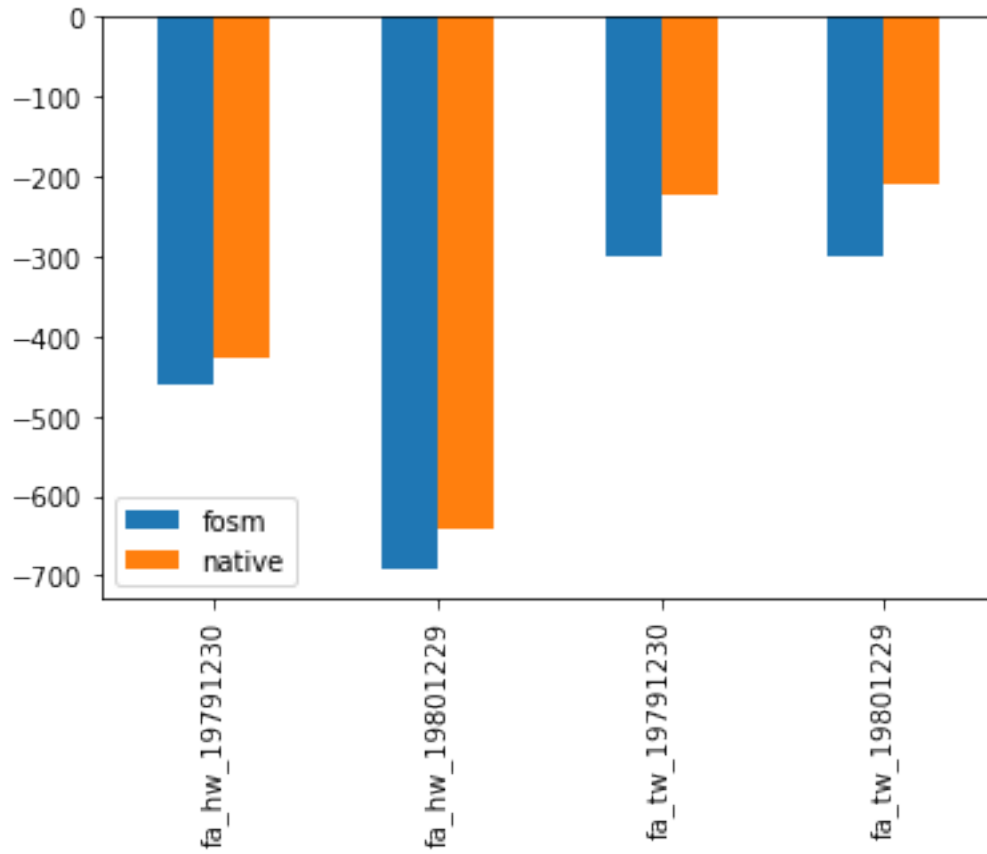
1.1.5 Opt under uncertainty part 2: ensemble-based chance constraints

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 [25]: 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 [26]: pr_std = obs_df.std().loc[pst.nnz_obs_names]
         pr_std

Out[26]: fa_hw_19791230     350.167840
         fa_hw_19801229     480.562490
         fa_tw_19791230     516.438506
         fa_tw_19801229     613.718801
         dtype: float64

In [27]: 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"))
```

11

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

```
In [28]: pyemu.os_utils.start_slaves(t_d,"pestpp-opt","freyberg_opt_uu2.pst",num_slaves=num_wo
```

```
In [29]: 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,:]
```

```
13.275434422681979
```

```
Out[29]:                       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   1.275434     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???

1.1.6   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 [30]: 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[30]: '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

```
In [31]: 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 [32]: pyemu.os_utils.run("pestpp-opt freyberg_opt_restart.pst",cwd=m_d)
```

```
In [33]: 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,:]
```

13.275434422681979

```
Out[33]:                       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   1.275434    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 [34]: 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
8.78881901939404

```
Out[34]:                       parnme    parval1   scale   offset
         parnme
         wf0200090016  wf0200090016   3.000000    1.0      0.0
         wf0200110013  wf0200110013   3.000000    1.0      0.0
         wf0200200014  wf0200200014   2.788819    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 [35]: 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]
```
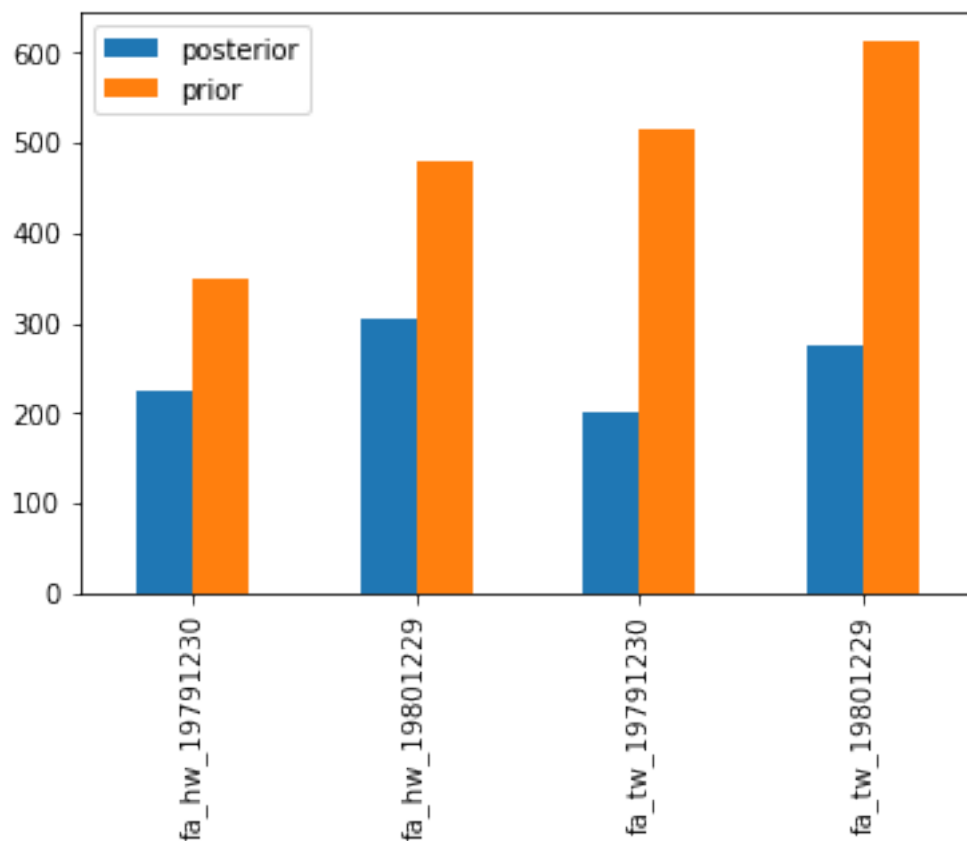
```
Out[35]: fa_hw_19791230    225.283936
         fa_hw_19801229    304.237446
         fa_tw_19791230    200.294474
         fa_tw_19801229    274.358924
         dtype: float64
```

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

```
In [36]: pd.DataFrame({"prior":pr_std,"posterior":pt_std}).plot(kind="bar")
```

```
Out[36]: <matplotlib.axes._subplots.AxesSubplot at 0x10e565358>
```

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 [37]: 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[37]: obsnme
         fa_hw_19791230     225.283936
         fa_hw_19801229     304.237446
         fa_tw_19791230     200.294474
         fa_tw_19801229     274.358924
         Name: weight, dtype: float64
```

```
In [38]: 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
9.301118835340247
```

```
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   3.000000     1.0      0.0
         wf0200260010   wf0200260010   0.000000     1.0      0.0
         wf0200290006   wf0200290006   0.000000     1.0      0.0
         wf0200340012   wf0200340012   0.301119     1.0      0.0
```

```
In [39]: pyemu.pst_utils.read_resfile(os.path.join(m_d,"freyberg_opt_restart.1.est+fosm.rei"))
```

```
Out[39]:                          name        group   measured     modelled      residual  \
         name
         fa_hw_19791230   fa_hw_19791230   less_than    -300.0  -394.604276    94.604276
         fa_hw_19801229   fa_hw_19801229   less_than    -300.0  -651.032416   351.032416
         fa_tw_19791230   fa_tw_19791230   less_than    -300.0  -441.613552   141.613552
         fa_tw_19801229   fa_tw_19801229   less_than    -300.0  -300.000000     0.000000


                            weight
         name
         fa_hw_19791230   225.283937
         fa_hw_19801229   304.237446
         fa_tw_19791230   200.294474
         fa_tw_19801229   274.358924
```

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 [40]: 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 [41]: tot_swgw = obs.loc[obs.obgnme=="flx_stream_","obsnme"]

In [42]: 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 [43]: obs_df.std().loc[pst.nnz_obs_names].plot(kind="bar")

Out[43]: <matplotlib.axes._subplots.AxesSubplot at 0x1821f19dd8>
```
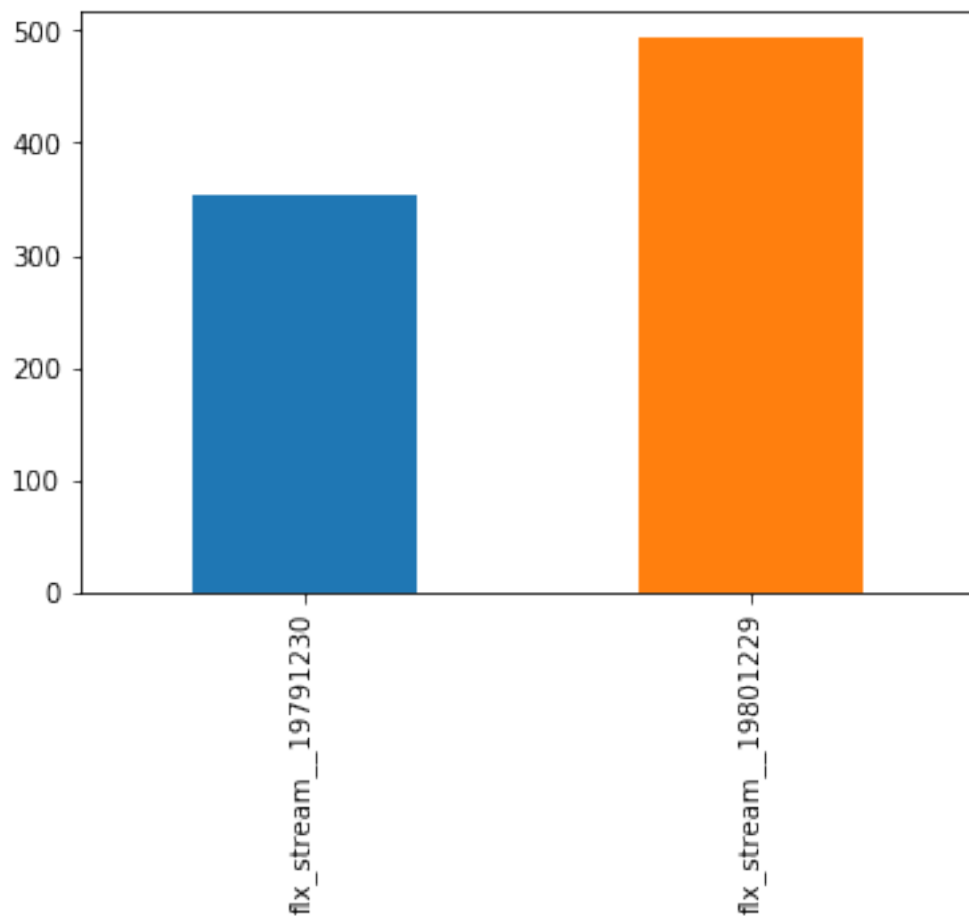
Since we want to find the most risk averse stance that is still feasible we will run a sweep of risk values:

```
In [44]: 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.par
             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 [45]: 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[45]: Text(0.5, 0, 'risk')
```
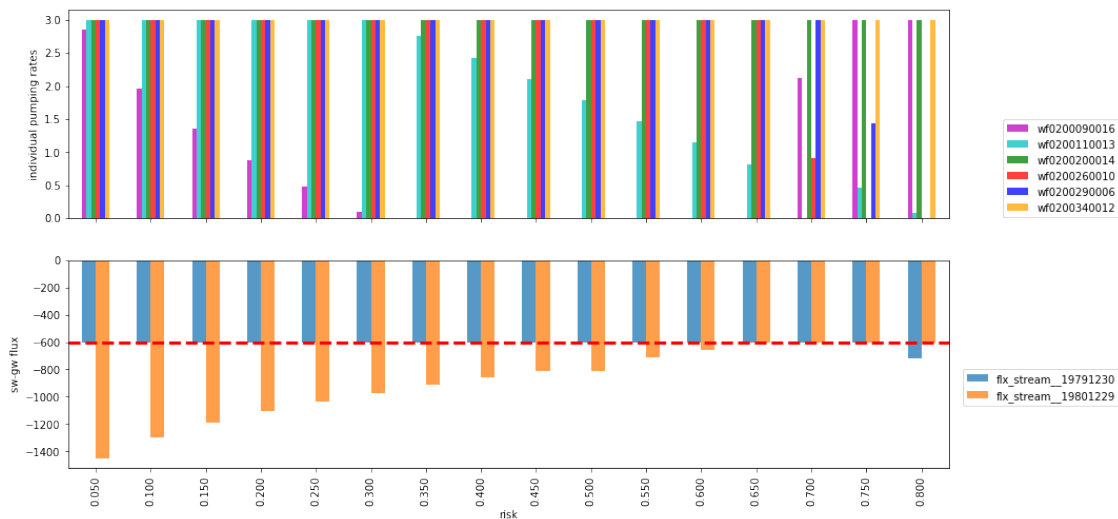


```
In [46]: m = flopy.modflow.Modflow.load("freyberg.nam",model_ws=t_d)
         wf_par = pst.parameter_data.loc[dvg_pars,:].copy()
         wf_par.loc[:,"k"] = wf_par.parnme.apply(lambda x: int(x[2:4]))
         wf_par.loc[:,"i"] = wf_par.parnme.apply(lambda x: int(x[4:8]))
         wf_par.loc[:,"j"] = 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")
```
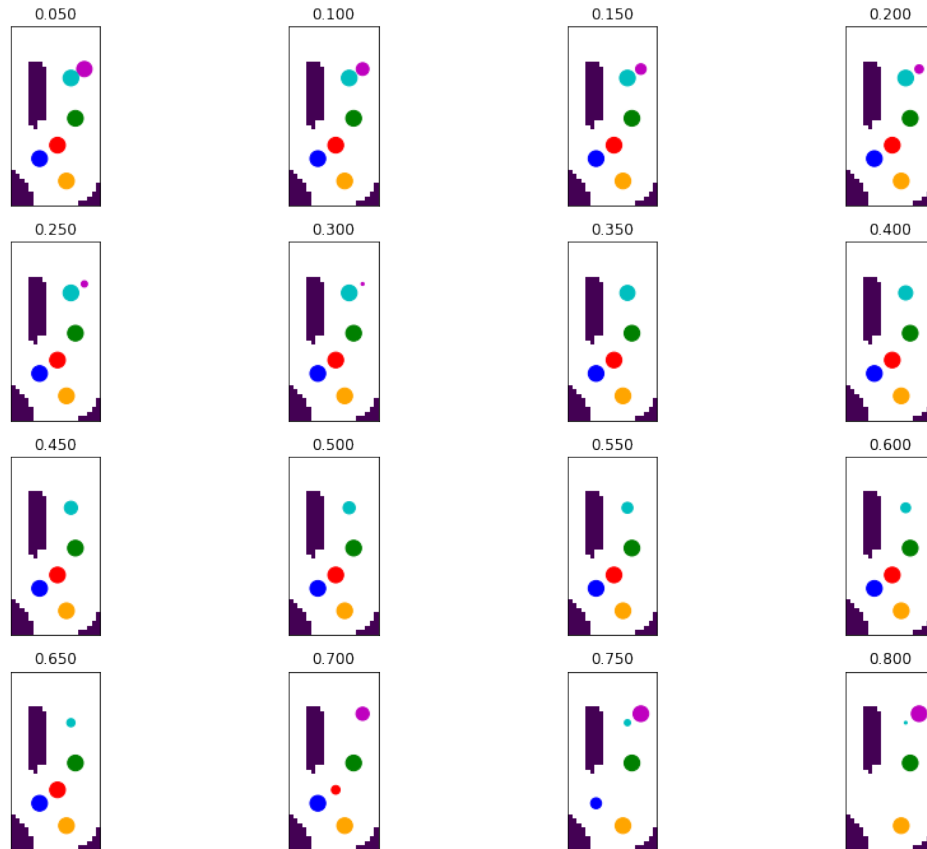
how about those figures!!!

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 [47]: 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[47]:   name   group   measured   modelled \
        name
        flx_stream__19791230 flx_stream__19791230 less_than   -600.0 -722.484605
        flx_stream__19801229 flx_stream__19801229 less_than   -600.0 -599.689146

                               residual   weight
        name
        flx_stream__19791230 122.484605   353.918119
        flx_stream__19801229   -0.310854   492.905194

In [48]: # load the actual model simulated outputs
        res_df_sim = pyemu.pst_utils.read_resfile(os.path.join(m_d,"freyberg_opt_restart.1.sir
        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[48]: [<matplotlib.lines.Line2D at 0x1824144a20>]
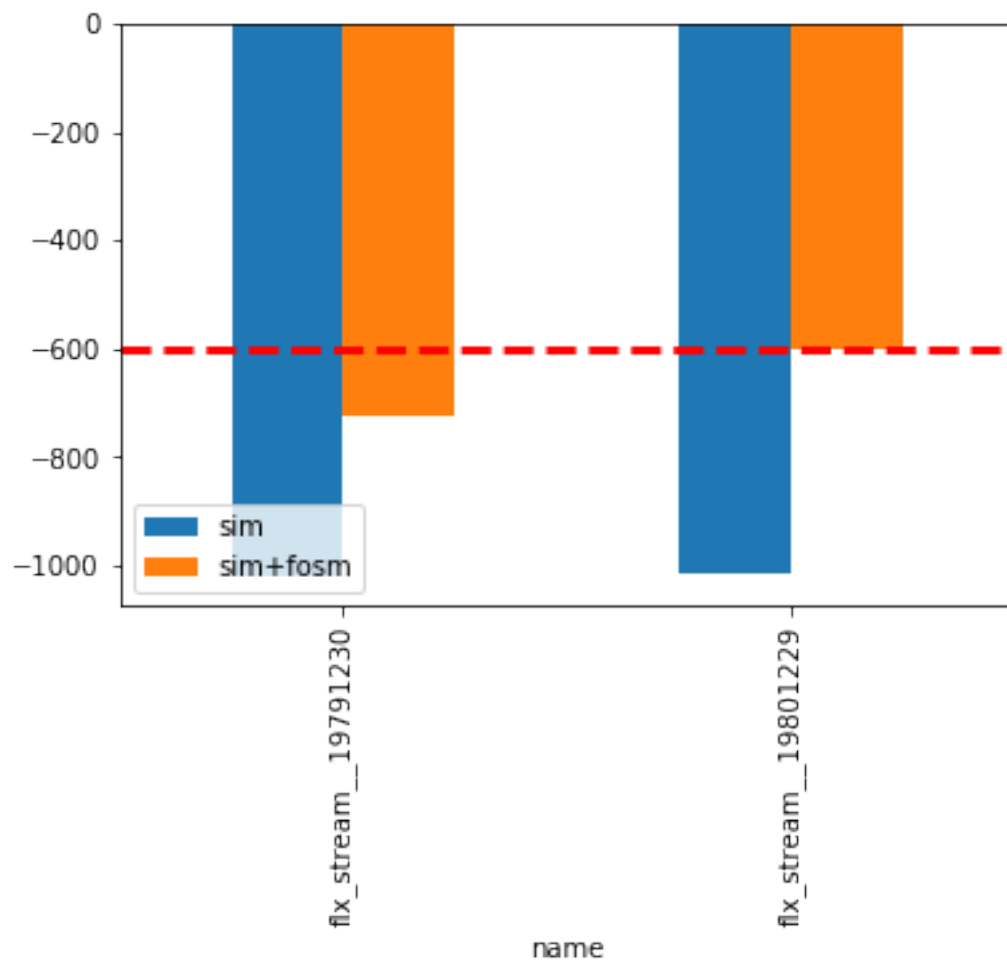
Here we can see the cost of uncertainty - we have to simulate a greater flux from gw to sw to make sure (e.g. be risk averse) that the flux from gw to sw is actually at least 600 m3/day

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!