pestpp-glm

May 18, 2019

1 PESTPP-GLM

In this notebook, we will run PESTPP-GLM in standard parameter estimation mode and regularization mode. In both cases, we will use the baked-in bayes-linear posterior monte carlo analysis to get posterior forecast PDFs. We will use the prior monte carlo outputs as the prior forecast PDF.

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 = 20
```

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

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

Out[4]:
```
                      type transform  count      initial value  \
gr_prsity5    gr_prsity5       log    705                  0
pp_strt0        pp_strt0       log     32                  0
flow                flow       log      1                  0
gr_vka3          gr_vka3       log    705                  0
pp_vka2          pp_vka2       log     32                  0
cn_sy7             cn_sy7       log      1                  0
pp_strt1        pp_strt1       log     32                  0
gr_vka4          gr_vka4       log    705                  0
```

cn_prsity6	cn_prsity6	log	1	0
gr_ss5	gr_ss5	log	705	0
pp_hk0	pp_hk0	log	32	0
pp_prsity1	pp_prsity1	log	32	0
cn_strt8	cn_strt8	log	1	0
pp_rech1	pp_rech1	log	32	0
cn_ss6	cn_ss6	log	1	0
cn_vka8	cn_vka8	log	1	0
gr_strt5	gr_strt5	log	705	0
pp_prsity0	pp_prsity0	log	32	0
cn_vka6	cn_vka6	log	1	0
cn_hk7	cn_hk7	log	1	0
pp_strt2	pp_strt2	log	32	0
cn_hk8	cn_hk8	log	1	0
welflux	welflux	log	2	0 to 0.176091
cn_prsity8	cn_prsity8	log	1	0
cn_hk6	cn_hk6	log	1	0
gr_prsity4	gr_prsity4	log	705	0
cn_rech5	cn_rech5	log	1	-0.39794
gr_ss3	gr_ss3	log	705	0
cn_strt7	cn_strt7	log	1	0
gr_rech2	gr_rech2	log	705	0
...	...	...	...	...
strk	strk	log	40	0
pp_ss1	pp_ss1	log	32	0
welflux_k02	welflux_k02	log	6	0
gr_hk4	gr_hk4	log	705	0
gr_sy5	gr_sy5	log	705	0
pp_ss2	pp_ss2	log	32	0
cn_prsity7	cn_prsity7	log	1	0
gr_prsity3	gr_prsity3	log	705	0
gr_sy3	gr_sy3	log	705	0
cn_sy8	cn_sy8	log	1	0
cn_strt6	cn_strt6	log	1	0
gr_strt4	gr_strt4	log	705	0
pp_ss0	pp_ss0	log	32	0
pp_prsity2	pp_prsity2	log	32	0
pp_hk1	pp_hk1	log	32	0
pp_vka0	pp_vka0	log	32	0
pp_rech0	pp_rech0	log	32	0
gr_strt3	gr_strt3	log	705	0
gr_ss4	gr_ss4	log	705	0
gr_sy4	gr_sy4	log	705	0
pp_sy0	pp_sy0	log	32	0
drncond_k00	drncond_k00	log	10	0
gr_hk5	gr_hk5	log	705	0
cn_vka7	cn_vka7	log	1	0
pp_sy1	pp_sy1	log	32	0

cn_sy6	cn_sy6	log	1	0
pp_hk2	pp_hk2	log	32	0
gr_vka5	gr_vka5	log	705	0
cn_ss8	cn_ss8	log	1	0
pp_vka1	pp_vka1	log	32	0

	upper bound	lower bound	standard deviation
gr_prsity5	0.176091	-0.30103	0.11928
pp_strt0	0.0211893	-0.0222764	0.0108664
flow	0.09691	-0.124939	0.0554622
gr_vka3	1	-1	0.5
pp_vka2	1	-1	0.5
cn_sy7	0.243038	-0.60206	0.211275
pp_strt1	0.0211893	-0.0222764	0.0108664
gr_vka4	1	-1	0.5
cn_prsity6	0.176091	-0.30103	0.11928
gr_ss5	1	-1	0.5
pp_hk0	1	-1	0.5
pp_prsity1	0.176091	-0.30103	0.11928
cn_strt8	0.0211893	-0.0222764	0.0108664
pp_rech1	0.0413927	-0.0457575	0.0217875
cn_ss6	1	-1	0.5
cn_vka8	1	-1	0.5
gr_strt5	0.0211893	-0.0222764	0.0108664
pp_prsity0	0.176091	-0.30103	0.11928
cn_vka6	1	-1	0.5
cn_hk7	1	-1	0.5
pp_strt2	0.0211893	-0.0222764	0.0108664
cn_hk8	1	-1	0.5
welflux	0.176091 to 0.30103	-0.30103 to 0	0.0752575 to 0.11928
cn_prsity8	0.176091	-0.30103	0.11928
cn_hk6	1	-1	0.5
gr_prsity4	0.176091	-0.30103	0.11928
cn_rech5	-0.09691	-1	0.225772
gr_ss3	1	-1	0.5
cn_strt7	0.0211893	-0.0222764	0.0108664
gr_rech2	0.0413927	-0.0457575	0.0217875
...	...	...	...
strk	2	-2	1
pp_ss1	1	-1	0.5
welflux_k02	1	-1	0.5
gr_hk4	1	-1	0.5
gr_sy5	0.243038	-0.60206	0.211275
pp_ss2	1	-1	0.5
cn_prsity7	0.176091	-0.30103	0.11928
gr_prsity3	0.176091	-0.30103	0.11928
gr_sy3	0.243038	-0.60206	0.211275
cn_sy8	0.243038	-0.60206	0.211275

```
cn_strt6          0.0211893   -0.0222764   0.0108664
gr_strt4          0.0211893   -0.0222764   0.0108664
pp_ss0                    1           -1         0.5
pp_prsity2         0.176091     -0.30103     0.11928
pp_hk1                    1           -1         0.5
pp_vka0                   1           -1         0.5
pp_rech0          0.0413927   -0.0457575   0.0217875
gr_strt3          0.0211893   -0.0222764   0.0108664
gr_ss4                    1           -1         0.5
gr_sy4             0.243038     -0.60206    0.211275
pp_sy0             0.243038     -0.60206    0.211275
drncond_k00               1           -1         0.5
gr_hk5                    1           -1         0.5
cn_vka7                   1           -1         0.5
pp_sy1             0.243038     -0.60206    0.211275
cn_sy6             0.243038     -0.60206    0.211275
pp_hk2                    1           -1         0.5
gr_vka5                   1           -1         0.5
cn_ss8                    1           -1         0.5
pp_vka1                   1           -1         0.5

[65 rows x 7 columns]
```

1.1.1 reduce the number of adjustable parameters

This is the painful part: we cant use 10K+ pars because we cant wait around for that many runs and then the linear algebra of factoring a 10k+ by 10K+ matrix is also difficult. So that means we need to fix a lot a parameters #frownyface

```
In [5]: par = pst.parameter_data
```

```
In [6]: # grid-scale pars
        gr_pars = par.loc[par.pargp.apply(lambda x: "gr" in x),"parnme"]
        par.loc[gr_pars,"partrans"] = "fixed"
        pst.npar_adj
```

```
Out[6]: 719
```

```
In [7]: # these are the sfr conductance parameters - Ive left all 40 adjustable
        # but if you uncomment this, it will tie them into 1 parameter effectively
        # strk_pars = par.loc[par.pargp=="strk","parnme"]
        # p1 = strk_pars.iloc[0]
        # par.loc[strk_pars.iloc[1:],"partrans"] = "tied"
        # par.loc[strk_pars.iloc[1:],"partied"] = p1
        pst.npar_adj
```

```
Out[7]: 719
```

```
In [8]: par.loc[par.pargp.apply(lambda x: "pp" in x),"pargp"].unique()
```

```
Out[8]: array(['pp_hk0', 'pp_hk1', 'pp_hk2', 'pp_prsity0', 'pp_prsity1',
               'pp_prsity2', 'pp_rech0', 'pp_rech1', 'pp_ss0', 'pp_ss1', 'pp_ss2',
               'pp_strt0', 'pp_strt1', 'pp_strt2', 'pp_sy0', 'pp_sy1', 'pp_sy2',
               'pp_vka0', 'pp_vka1', 'pp_vka2'], dtype=object)
```

Fix the storage pilot points - we still have layer-scale storage pars adjustable

```
In [9]: #s_pars = par.loc[par.pargp.apply(lambda x: "pp" in x and ("ss" in x or "sy" in x)),"p
        #par.loc[s_pars,"partrans"] = "fixed"
        pst.npar_adj
```

```
Out[9]: 719
```

```
In [10]: adj_par = par.loc[par.partrans=="log",:]
         adj_par.pargp.value_counts().sort_values()
```

```
Out[10]: cn_strt7         1
         cn_prsity6       1
         cn_strt8         1
         cn_vka8          1
         flow             1
         cn_ss6           1
         cn_vka6          1
         cn_ss8           1
         cn_hk6           1
         cn_sy7           1
         cn_sy8           1
         cn_hk7           1
         cn_prsity8       1
         cn_sy6           1
         cn_hk8           1
         cn_rech4         1
         cn_ss7           1
         cn_prsity7       1
         cn_strt6         1
         cn_vka7          1
         cn_rech5         1
         welflux          2
         welflux_k02      6
         drncond_k00     10
         pp_strt1        32
         pp_prsity0      32
         pp_hk2          32
         pp_sy0          32
         pp_sy2          32
         pp_vka2         32
         pp_strt2        32
         pp_ss1          32
         pp_prsity1      32
```

```
pp_ss2          32
pp_hk0          32
pp_prsity2      32
pp_hk1          32
pp_vka0         32
pp_rech0        32
pp_strt0        32
pp_rech1        32
pp_vka1         32
pp_sy1          32
pp_ss0          32
strk            40
Name: pargp, dtype: int64
```

fix the future recharge pilot points, vka in layers 1 and 3 and the initial condition pilot points (we still have layer-scale pars for each of these types)

```
In [11]: fi_grps = ["pp_rech1","pp_vka0","pp_vka2","pp_strt0","pp_strt1","pp_strt2"]
         par.loc[par.pargp.apply(lambda x: x in fi_grps),"partrans"] = "fixed"
         pst.npar_adj
```

```
Out[11]: 527
```

Ok, thats better. . . so lets run PESTPP-GLM. We will use a single "base parameter" jacobian matrix as the basis for 6 super parameter iterations. Then we will draw 100 realizations from the FOSM posterior parameter covariance matrix and run those 100 realizations to get the psoterior forecast PDFs

```
In [12]: pst.control_data.noptmax = 3
         pst.pestpp_options["n_iter_base"] = -1
         pst.pestpp_options["n_iter_super"] = 3
         pst.pestpp_options["num_reals"] = 50 # this is how many ies uses
         pst.pestpp_options["parcov"] = "prior_cov.jcb"
         pst.write(os.path.join(t_d,"freyberg_pp.pst"))
```

```
noptmax:3, npar_adj:527, nnz_obs:14
```

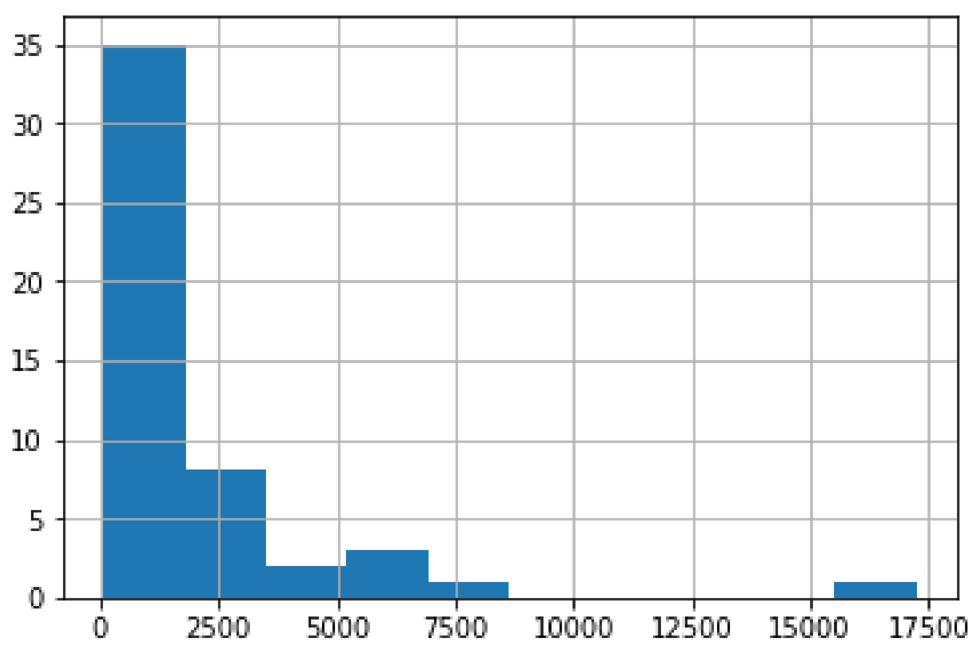
```
In [13]: pyemu.os_utils.start_slaves(t_d,"pestpp-glm","freyberg_pp.pst",num_slaves=num_workers
                                     master_dir=m_d)
```

```
In [14]: df = df=pd.read_csv(os.path.join(m_d,"freyberg_pp.post.obsen.csv"),index_col=0)
         oe = pyemu.ObservationEnsemble.from_dataframe(pst=pst,df=df)
```

```
In [15]: ax = oe.phi_vector.hist()#bins=np.linspace(0,100,20))
         oe.phi_vector.sort_values().iloc[:20]
```

```
Out[15]: real_name
         11     67.311123
```

```
19     73.629202
48     80.294490
37     85.556290
39    130.363406
46    142.101852
16    170.446318
34    192.605624
33    206.148352
24    220.418561
29    254.451689
1     255.306658
17    289.671776
26    398.593623
7     428.985089
45    516.951351
44    570.947286
38    664.273902
49    679.494764
23    681.123367
dtype: float64
```



Here we see the distribution of phi values across the 100 posterior realizations. Should we accept all of these??? The theoretical phi we should accept is number of nonzero obs (14).

To get a "posterior" ensemble, we need to throw out the realizations with large phi - lets just take the 20 best:

```
In [16]: oe_pt = oe.loc[oe.phi_vector.sort_values().index[:20],:] #just take the 20 lowest phi
```

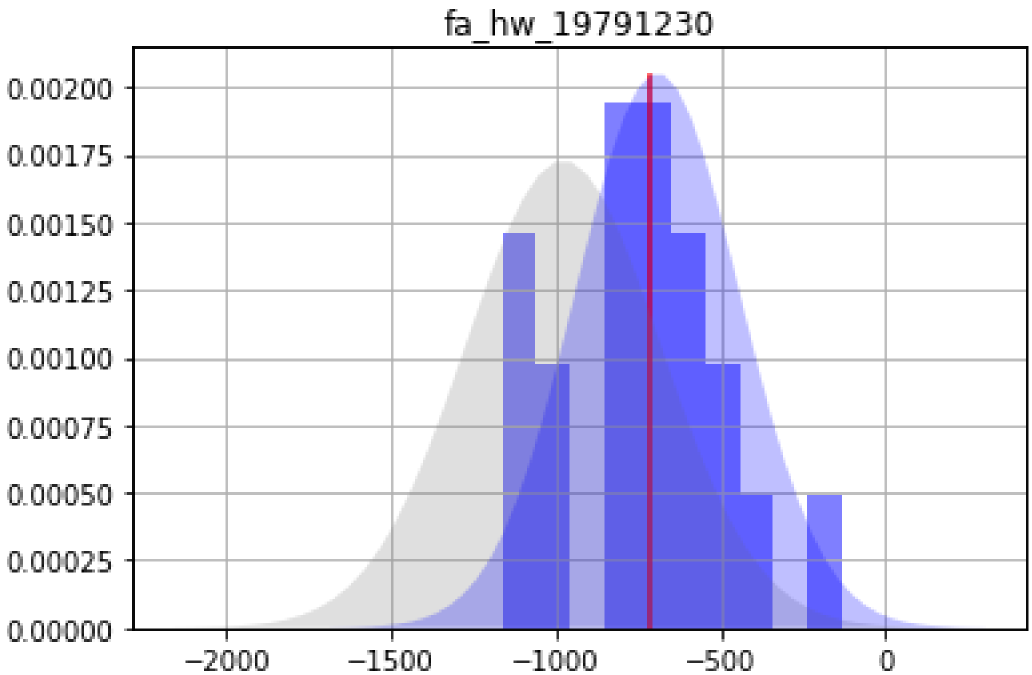
We can also load and plot the FOSM forecast results along side of the ensemble results:

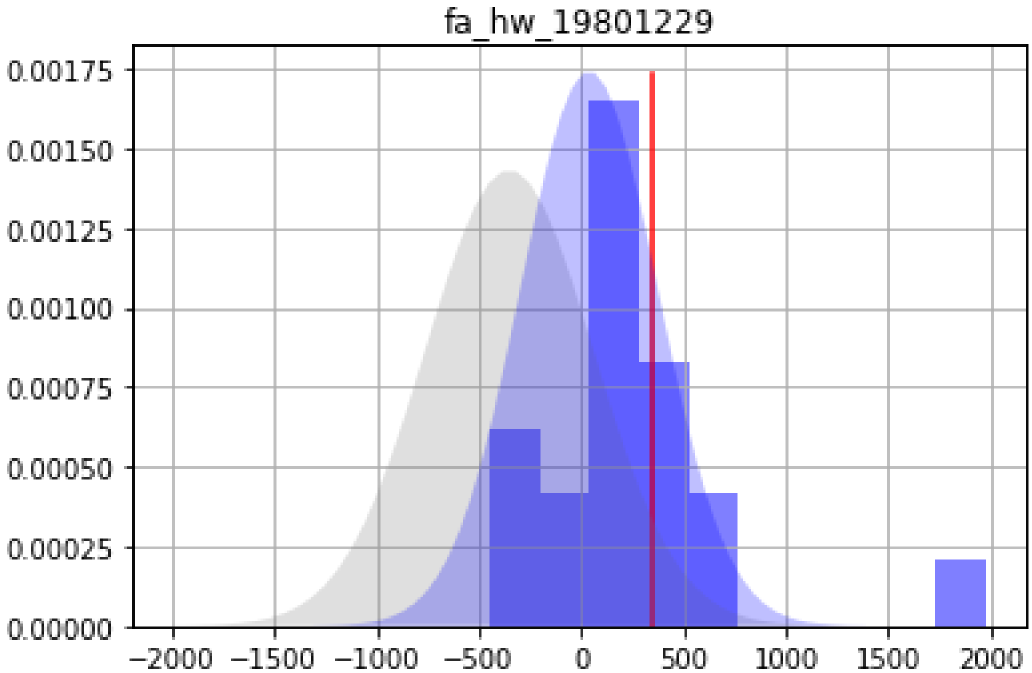
In [17]:
```python
f_df = pd.read_csv(os.path.join(m_d,"freyberg_pp.pred.usum.csv"),index_col=0)
f_df.index = f_df.index.map(str.lower)
f_df
```

Out[17]:
```
                     prior_mean  prior_stdev  prior_lower_bound  \
name
fa_hw_19791230        -977.2390    295.32800         -1567.8900
fa_hw_19801229        -351.2160    409.77000         -1170.7600
fa_tw_19791230        -453.0330    409.35100         -1271.7400
fa_tw_19801229         108.9600    506.73200          -904.5040
hds_00_013_002_000      39.6102      3.96314            31.6840
hds_00_013_002_001      38.3838      4.05782            30.2681
part_status              2.0000      0.00000             2.0000
part_time              907.7020    570.98600          -234.2690

                     prior_upper_bound  post_mean  post_stdev  \
name
fa_hw_19791230               -386.5840  -691.3690  248.764000
fa_hw_19801229                468.3240    38.8612  336.875000
fa_tw_19791230                365.6690  -315.6270  172.537000
fa_tw_19801229               1122.4200   335.7690  265.523000
hds_00_013_002_000             47.5365    37.6724    0.283577
hds_00_013_002_001             46.4994    36.4533    0.691648
part_status                     2.0000     2.0000    0.000000
part_time                    2049.6700   660.4670  437.861000

                     post_lower_bound  post_upper_bound
name
fa_hw_19791230             -1188.9000         -193.8410
fa_hw_19801229              -634.8880          712.6110
fa_tw_19791230              -660.7020           29.4469
fa_tw_19801229              -195.2760          866.8150
hds_00_013_002_000            37.1052           38.2395
hds_00_013_002_001            35.0700           37.8366
part_status                    2.0000            2.0000
part_time                   -215.2550         1536.1900
```

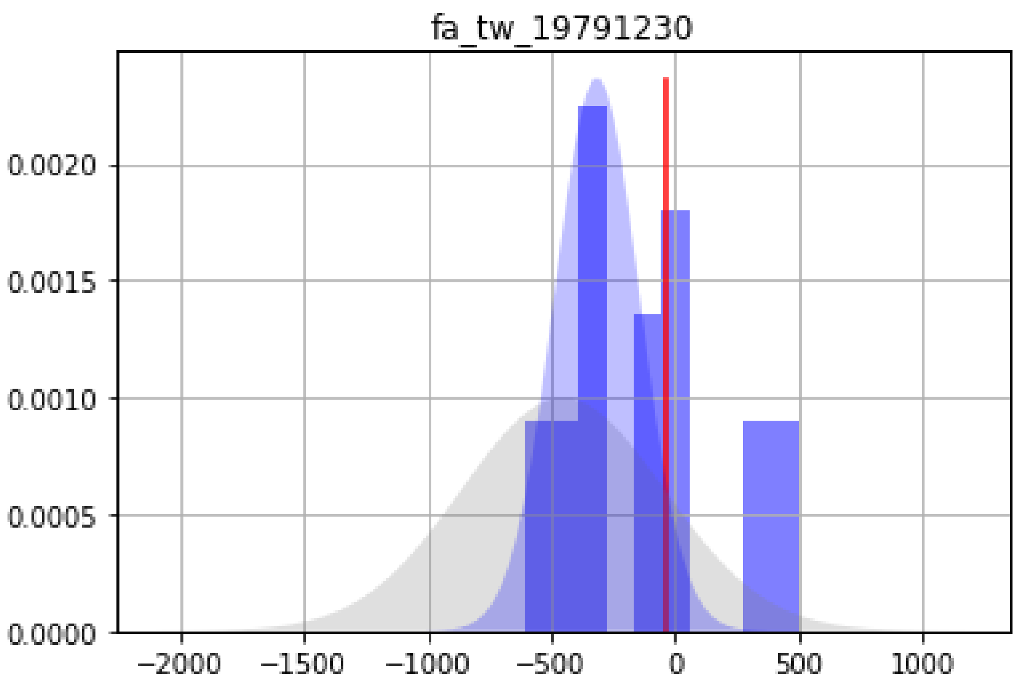
In [18]:
```python
obs = pst.observation_data
fnames = pst.pestpp_options["forecasts"].split(",")
for forecast in fnames:
    ax = plt.subplot(111)
    oe_pt.loc[:,forecast].hist(ax=ax,color="b",alpha=0.5,normed=True)
    ax.plot([obs.loc[forecast,"obsval"],obs.loc[forecast,"obsval"]],ax.get_ylim(),"r"
    axt = plt.twinx()
    x,y = pyemu.plot_utils.gaussian_distribution(f_df.loc[forecast,"prior_mean"],f_df
    axt.fill_between(x,0,y,facecolor="0.5",alpha=0.25)
```

```
x,y = pyemu.plot_utils.gaussian_distribution(f_df.loc[forecast,"post_mean"],f_df.l
axt.fill_between(x,0,y,facecolor="b",alpha=0.25)
axt.set_ylim(0,axt.get_ylim()[1])
axt.set_yticks([])
ax.set_title(forecast)
plt.show()
```

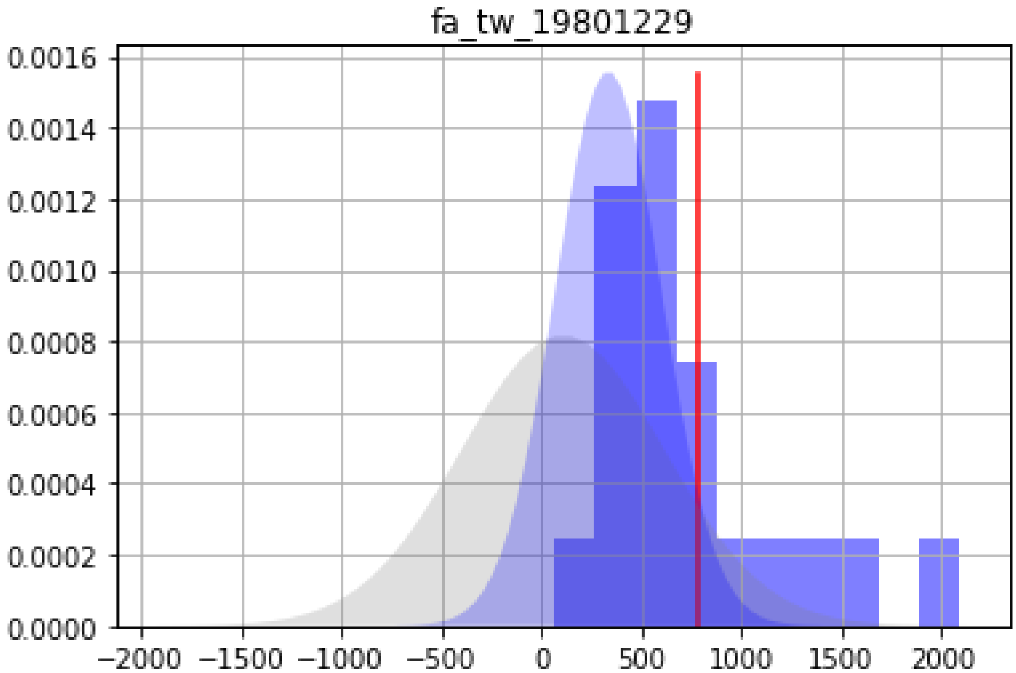


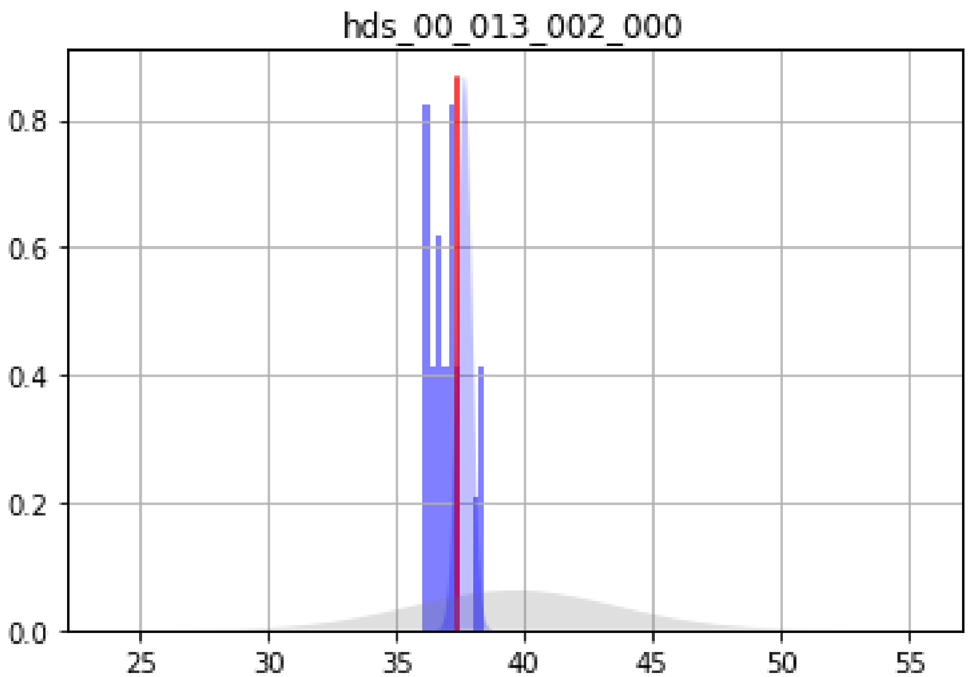


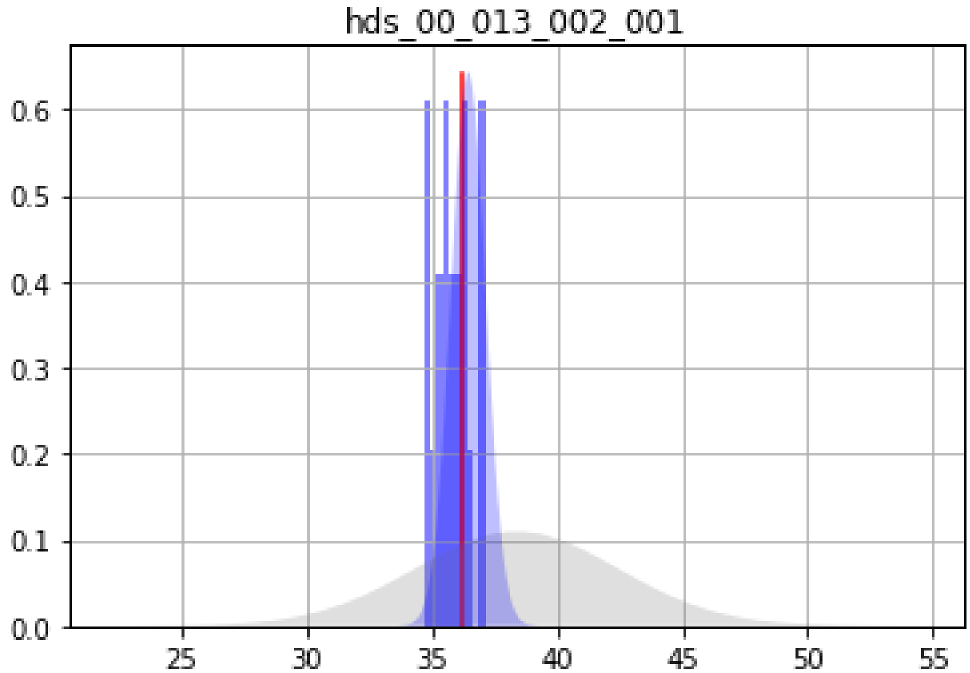
fa_hw_19801229
0.00175
0.00150
0.00125
0.00100
0.00075
0.00050
0.00025
0.00000
−2000
−1500
−1000
−500
0
500
1000
1500
2000

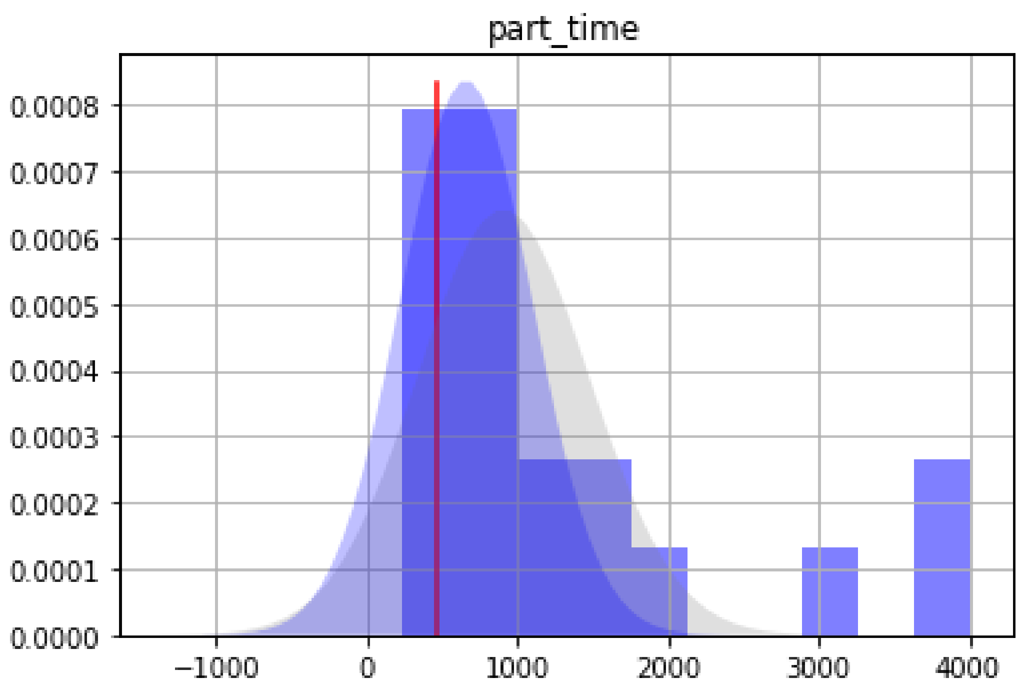


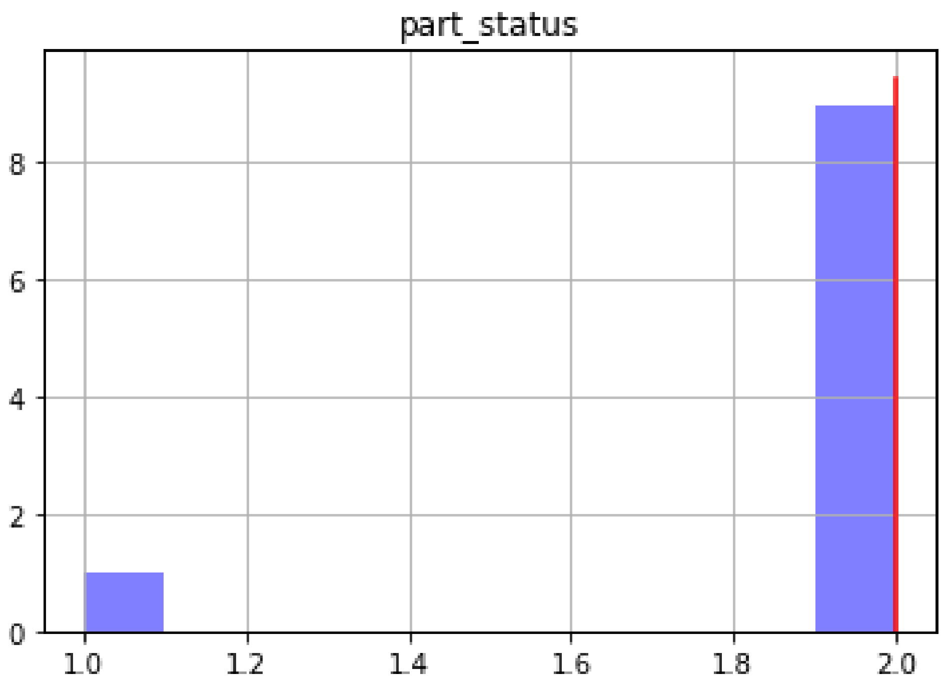
fa_tw_19791230
0.0020
0.0015
0.0010
0.0005
0.0000
−2000
−1500
−1000
−500
0
500
1000


fa_tw_19801229
0.0016
0.0014
0.0012
0.0010
0.0008
0.0006
0.0004
0.0002
0.0000
−2000
−1500
−1000
−500
0
500
1000
1500
2000


hds_00_013_002_000
0.8
0.6
0.4
0.2
0.0
25
30
35
40
45
50
55


hds_00_013_002_001
0.0
0.1
0.2
0.3
0.4
0.5
0.6
25
30
35
40
45
50
55


part_time
0.0000
0.0001
0.0002
0.0003
0.0004
0.0005
0.0006
0.0007
0.0008
−1000
0
1000
2000
3000
4000



1.1.2 Setup of Tikhonov regularization

Now lets setup and use some formal regularization to bring the final phi up to around 14. We will use first-order regularization based on the covariance matrix we build earlier:

```
In [19]: cov = pyemu.Cov.from_binary(os.path.join(t_d,"prior_cov.jcb"))
```

```
new binary format detected...
```

```
In [20]: pyemu.helpers.first_order_pearson_tikhonov(pst,cov)
```

```
getting CC matrix
processing
```

```
In [21]: pst.prior_information.head()
```

```
Out[21]:                                                   equation    obgnme  \
         pilbl
         pcc_1  1.0 * log(dc0000390005) - 1.0 * log(dc0000390006) = 0.0  regul_cc
         pcc_2  1.0 * log(dc0000390005) - 1.0 * log(dc0000390007) = 0.0  regul_cc
         pcc_3  1.0 * log(dc0000390005) - 1.0 * log(dc0000390008) = 0.0  regul_cc
         pcc_4  1.0 * log(dc0000390005) - 1.0 * log(dc0000390009) = 0.0  regul_cc
         pcc_5  1.0 * log(dc0000390005) - 1.0 * log(dc0000390010) = 0.0  regul_cc
```

```
       pilbl    weight
pilbl
pcc_1  pcc_1  0.904837
pcc_2  pcc_2  0.818731
pcc_3  pcc_3  0.740818
pcc_4  pcc_4  0.670320
pcc_5  pcc_5  0.606531
```

In [22]:
```
shutil.copy2(os.path.join(m_d,"freyberg_pp.jcb"),os.path.join(t_d,"restart_pp.jcb"))
```

Out[22]:
```
'template/restart_pp.jcb'
```

In [23]:
```
pst.pestpp_options["base_jacobian"] = "restart_pp.jcb"
pst.reg_data.phimlim = pst.nnz_obs
pst.reg_data.phimaccept = pst.reg_data.phimlim * 1.1
pst.write(os.path.join(t_d,"freyberg_pp.pst"))
```

```
noptmax:3, npar_adj:527, nnz_obs:14
```

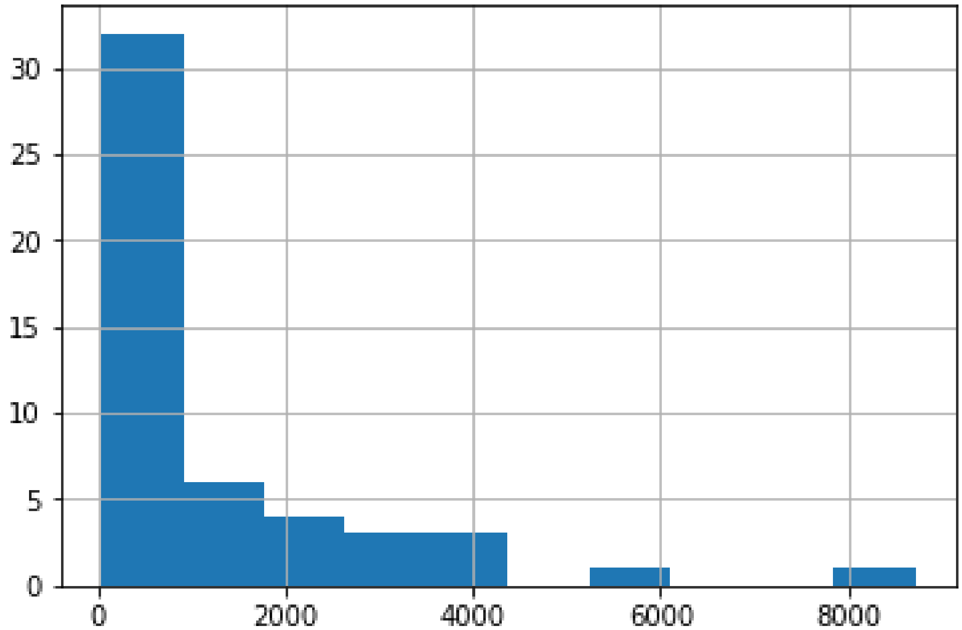
In [24]:
```
pyemu.os_utils.start_slaves(t_d,"pestpp-glm","freyberg_pp.pst",num_slaves=num_workers
                            master_dir=m_d)
```

In [25]:
```
df = df=pd.read_csv(os.path.join(m_d,"freyberg_pp.post.obsen.csv"),index_col=0)
oe = pyemu.ObservationEnsemble.from_dataframe(pst=pst,df=df)
```

In [26]:
```
ax = oe.phi_vector.hist()#bins=np.linspace(0,100,20))
oe.phi_vector.sort_values().iloc[:20]
```

Out[26]:
```
real_name
48     36.238820
38     54.829565
11     63.978008
37    103.284082
46    109.420095
19    132.244209
26    140.618000
34    166.380438
17    174.431787
16    191.814022
24    201.539107
1     203.762385
39    233.843119
33    236.361174
5     270.972756
47    308.716219
29    395.603897
44    450.205197
```

```
6     469.426236
49    477.567389
dtype: float64
```



Same as before, to get a "posterior" ensemble, we need to throw out the realizations with large phi - lets just take the 20 best:

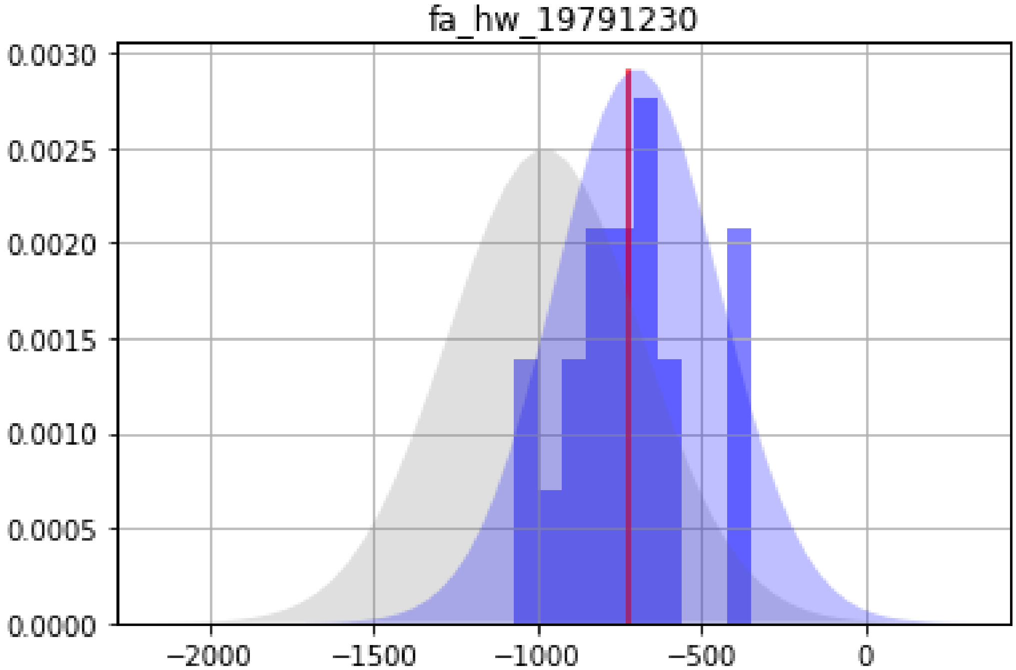
```
In [27]: oe_pt = oe.loc[oe.phi_vector.sort_values().index[:20],:]
```

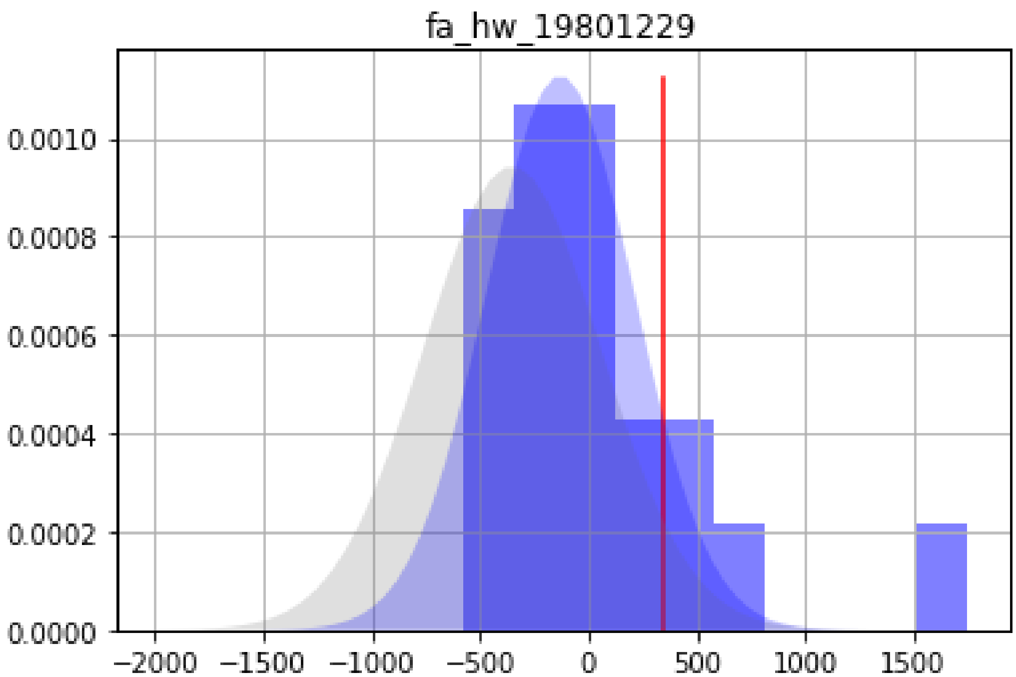
```
In [28]: f_df = pd.read_csv(os.path.join(m_d,"freyberg_pp.pred.usum.csv"),index_col=0)
         f_df.index = f_df.index.map(str.lower)
         f_df
```

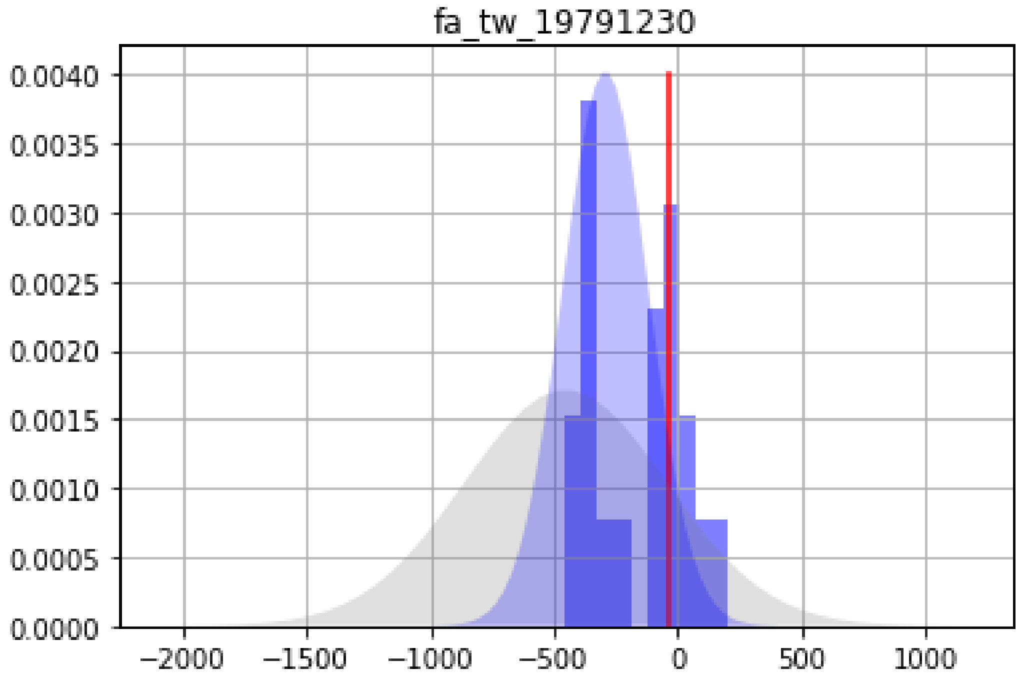
```
Out[28]:                        prior_mean  prior_stdev  prior_lower_bound  \
         name
         fa_hw_19791230          -977.2390    295.32800         -1567.8900
         fa_hw_19801229          -351.2160    409.77000         -1170.7600
         fa_tw_19791230          -453.0330    409.35100         -1271.7400
         fa_tw_19801229           108.9600    506.73200          -904.5040
         hds_00_013_002_000        39.6102      3.96314            31.6840
         hds_00_013_002_001        38.3838      4.05782            30.2681
         part_status                2.0000      0.00000             2.0000
         part_time                907.7020    570.98600          -234.2690

                                prior_upper_bound  post_mean  post_stdev  \
         name
         fa_hw_19791230                 -386.5840  -696.3770  252.671000
```

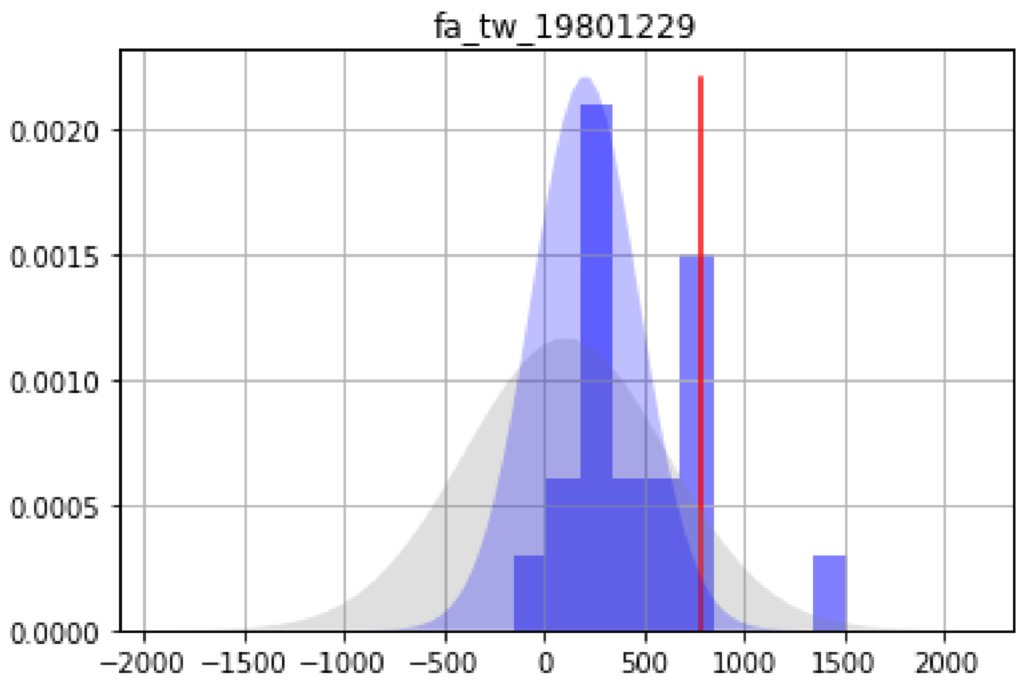
```
fa_hw_19801229              468.3240  -128.8820  342.901000
fa_tw_19791230              365.6690  -292.7330  174.083000
fa_tw_19801229             1122.4200   206.5750  267.003000
hds_00_013_002_000           47.5365    37.8527    0.291081
hds_00_013_002_001           46.4994    36.9254    0.694710
part_status                   2.0000     2.0000    0.000000
part_time                  2049.6700   900.1010  438.233000

                    post_lower_bound  post_upper_bound
name
fa_hw_19791230            -1201.7200         -191.0340
fa_hw_19801229             -814.6840          556.9200
fa_tw_19791230             -640.8980           55.4319
fa_tw_19801229             -327.4310          740.5810
hds_00_013_002_000           37.2706           38.4349
hds_00_013_002_001           35.5360           38.3148
part_status                   2.0000            2.0000
part_time                    23.6357         1776.5700
```

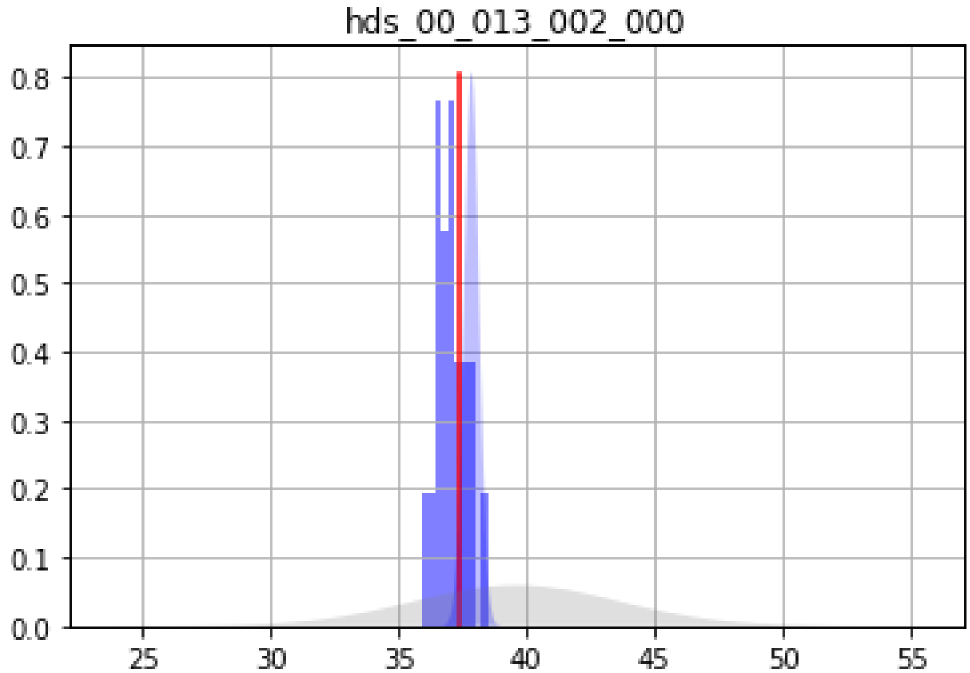
In [29]:
```
obs = pst.observation_data
fnames = pst.pestpp_options["forecasts"].split(",")
for forecast in fnames:
    ax = plt.subplot(111)
    oe_pt.loc[:,forecast].hist(ax=ax,color="b",alpha=0.5,normed=True)
    ax.plot([obs.loc[forecast,"obsval"],obs.loc[forecast,"obsval"]],ax.get_ylim(),"r"
    axt = plt.twinx()
    x,y = pyemu.plot_utils.gaussian_distribution(f_df.loc[forecast,"prior_mean"],f_df
    axt.fill_between(x,0,y,facecolor="0.5",alpha=0.25)
    x,y = pyemu.plot_utils.gaussian_distribution(f_df.loc[forecast,"post_mean"],f_df.
    axt.fill_between(x,0,y,facecolor="b",alpha=0.25)
    axt.set_ylim(0,axt.get_ylim()[1])
    axt.set_yticks([])
    ax.set_title(forecast)
    plt.show()
```

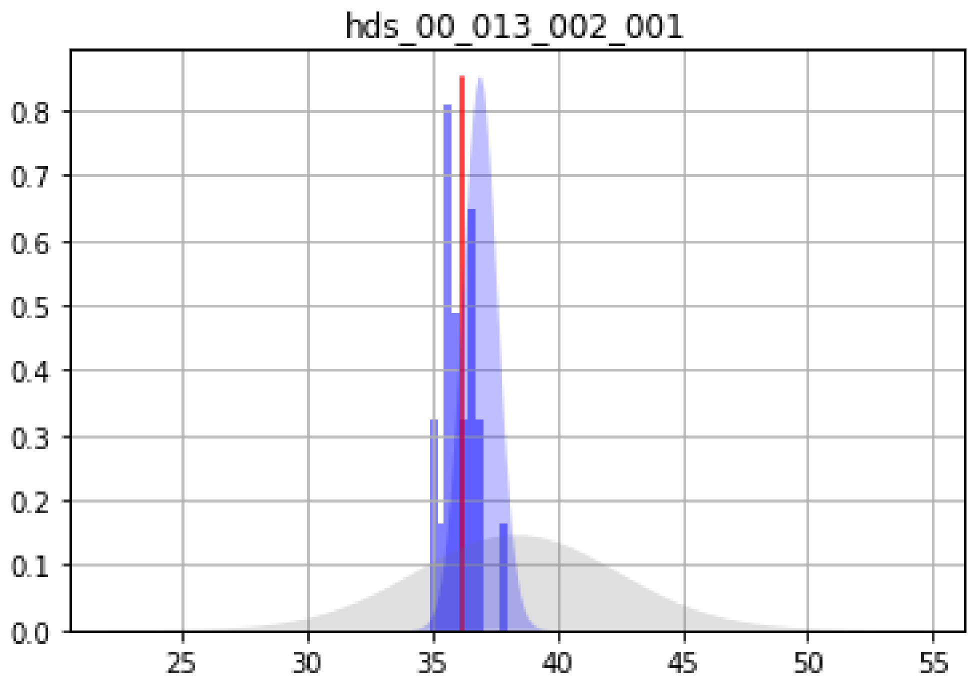

fa_hw_19791230
0.0030
0.0025
0.0020
0.0015
0.0010
0.0005
0.0000
−2000
−1500
−1000
−500
0

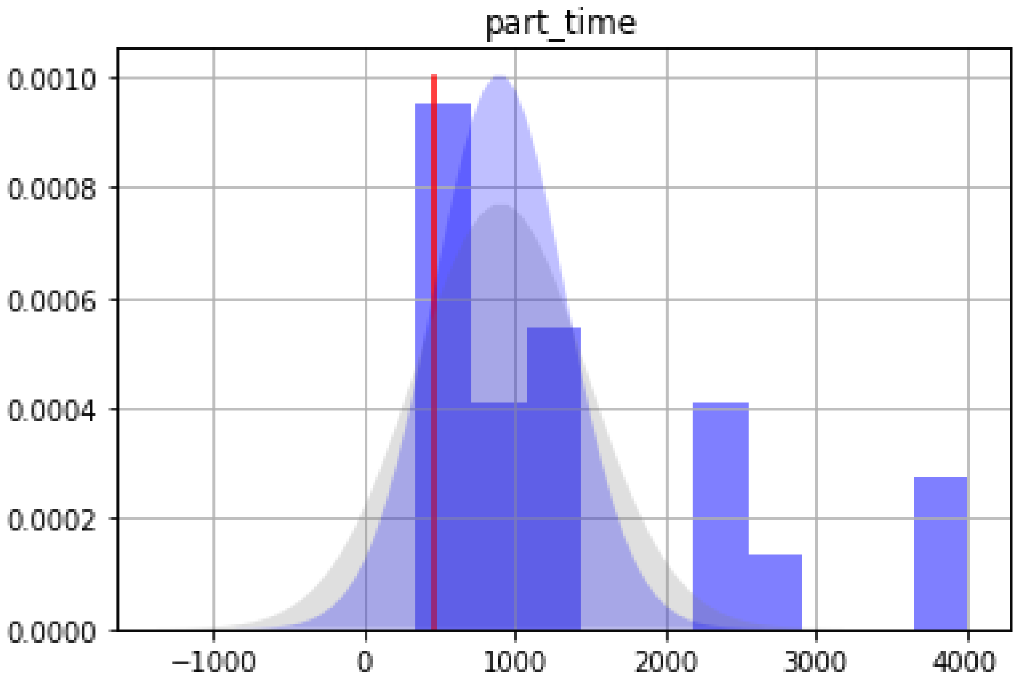

fa_hw_19801229
0.0010
0.0008
0.0006
0.0004
0.0002
0.0000
−2000
−1500
−1000
−500
0
500
1000
1500

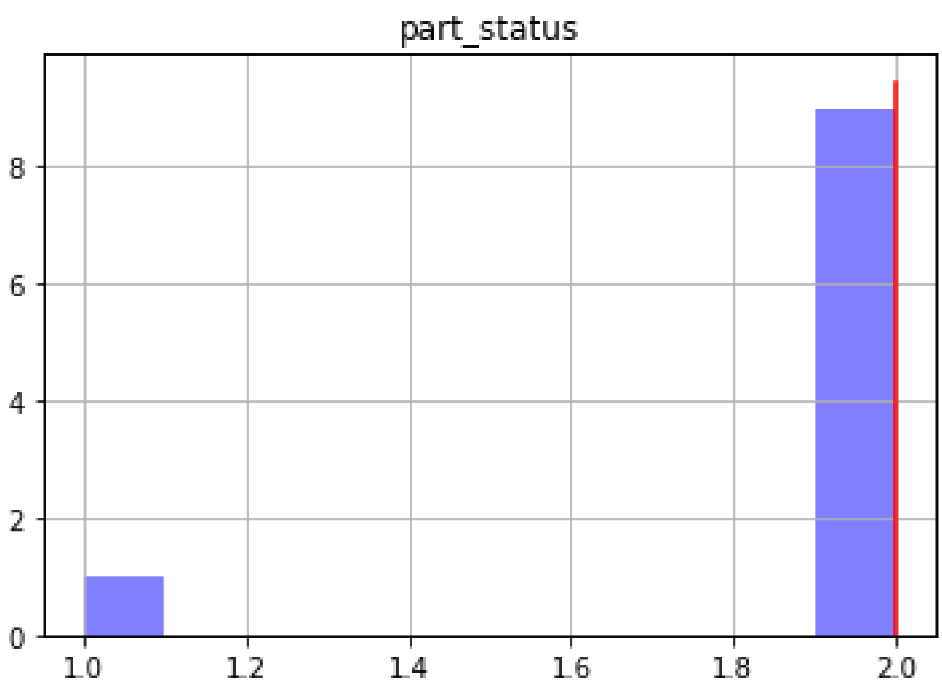

fa_tw_19791230
0.0040
0.0035
0.0030
0.0025
0.0020
0.0015
0.0010
0.0005
0.0000
−2000
−1500
−1000
−500
0
500
1000


fa_tw_19801229
0.0020
0.0015
0.0010
0.0005
0.0000
−2000
−1500
−1000
−500
0
500
1000
1500
2000


hds_00_013_002_000
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0.0
25
30
35
40
45
50
55


hds_00_013_002_001
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0.0
25
30
35
40
45
50
55


part_time
0.0010
0.0008
0.0006
0.0004
0.0002
0.0000
−1000
0
1000
2000
3000
4000


part_status
8
6
4
2
0
1.0
1.2
1.4
1.6
1.8
2.0