pestpp-glm

May 2, 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 flopy
import pyemu
```

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

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

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

Out[3]:
```
                      type transform  count      initial value  \
pp_strt2          pp_strt2       log     32                  0
gr_rech2          gr_rech2       log    705                  0
cn_strt8          cn_strt8       log      1                  0
gr_vka4             gr_vka4       log    705                  0
gr_ss3               gr_ss3       log    705                  0
pp_hk0               pp_hk0       log     32                  0
cn_hk7               cn_hk7       log      1                  0
pp_rech0          pp_rech0       log     32                  0
cn_hk6               cn_hk6       log      1                  0
welflux             welflux       log      2      0 to 0.176091
gr_hk5               gr_hk5       log    705                  0
cn_sy8               cn_sy8       log      1                  0
gr_strt3          gr_strt3       log    705                  0
```

pp_ss0	pp_ss0	log	32	0
gr_ss5	gr_ss5	log	705	0
gr_vka5	gr_vka5	log	705	0
pp_rech1	pp_rech1	log	32	0
gr_sy4	gr_sy4	log	705	0
pp_strt1	pp_strt1	log	32	0
pp_vka1	pp_vka1	log	32	0
pp_prsity1	pp_prsity1	log	32	0
gr_sy3	gr_sy3	log	705	0
cn_prsity8	cn_prsity8	log	1	0
pp_hk1	pp_hk1	log	32	0
cn_hk8	cn_hk8	log	1	0
gr_strt5	gr_strt5	log	705	0
pp_sy0	pp_sy0	log	32	0
cn_strt7	cn_strt7	log	1	0
gr_ss4	gr_ss4	log	705	0
cn_ss7	cn_ss7	log	1	0
...	...	...	...	...
pp_sy1	pp_sy1	log	32	0
cn_vka6	cn_vka6	log	1	0
gr_hk4	gr_hk4	log	705	0
cn_prsity7	cn_prsity7	log	1	0
flow	flow	log	1	0
gr_prsity4	gr_prsity4	log	705	0
welflux_k02	welflux_k02	log	6	0
cn_vka8	cn_vka8	log	1	0
cn_ss6	cn_ss6	log	1	0
cn_rech4	cn_rech4	log	1	0
pp_ss2	pp_ss2	log	32	0
gr_rech3	gr_rech3	log	705	0
pp_strt0	pp_strt0	log	32	0
pp_prsity0	pp_prsity0	log	32	0
cn_prsity6	cn_prsity6	log	1	0
gr_strt4	gr_strt4	log	705	0
cn_rech5	cn_rech5	log	1	-0.39794
cn_strt6	cn_strt6	log	1	0
cn_ss8	cn_ss8	log	1	0
gr_hk3	gr_hk3	log	705	0
cn_sy6	cn_sy6	log	1	0
gr_prsity3	gr_prsity3	log	705	0
pp_vka0	pp_vka0	log	32	0
gr_sy5	gr_sy5	log	705	0
pp_hk2	pp_hk2	log	32	0
pp_vka2	pp_vka2	log	32	0
pp_sy2	pp_sy2	log	32	0
pp_prsity2	pp_prsity2	log	32	0
strk	strk	log	40	0
gr_vka3	gr_vka3	log	705	0

	upper bound	lower bound	standard deviation
pp_strt2	0.0211893	-0.0222764	0.0108664
gr_rech2	0.0413927	-0.0457575	0.0217875
cn_strt8	0.0211893	-0.0222764	0.0108664
gr_vka4	1	-1	0.5
gr_ss3	1	-1	0.5
pp_hk0	1	-1	0.5
cn_hk7	1	-1	0.5
pp_rech0	0.0413927	-0.0457575	0.0217875
cn_hk6	1	-1	0.5
welflux	0.176091 to 0.30103	-0.30103 to 0	0.0752575 to 0.11928
gr_hk5	1	-1	0.5
cn_sy8	0.243038	-0.60206	0.211275
gr_strt3	0.0211893	-0.0222764	0.0108664
pp_ss0	1	-1	0.5
gr_ss5	1	-1	0.5
gr_vka5	1	-1	0.5
pp_rech1	0.0413927	-0.0457575	0.0217875
gr_sy4	0.243038	-0.60206	0.211275
pp_strt1	0.0211893	-0.0222764	0.0108664
pp_vka1	1	-1	0.5
pp_prsity1	0	-1	0.25
gr_sy3	0.243038	-0.60206	0.211275
cn_prsity8	0	-1	0.25
pp_hk1	1	-1	0.5
cn_hk8	1	-1	0.5
gr_strt5	0.0211893	-0.0222764	0.0108664
pp_sy0	0.243038	-0.60206	0.211275
cn_strt7	0.0211893	-0.0222764	0.0108664
gr_ss4	1	-1	0.5
cn_ss7	1	-1	0.5
...	...	...	...
pp_sy1	0.243038	-0.60206	0.211275
cn_vka6	1	-1	0.5
gr_hk4	1	-1	0.5
cn_prsity7	0	-1	0.25
flow	0.09691	-0.124939	0.0554622
gr_prsity4	0	-1	0.25
welflux_k02	1	-1	0.5
cn_vka8	1	-1	0.5
cn_ss6	1	-1	0.5
cn_rech4	0.0791812	-0.09691	0.0440228
pp_ss2	1	-1	0.5
gr_rech3	0.0413927	-0.0457575	0.0217875
pp_strt0	0.0211893	-0.0222764	0.0108664
pp_prsity0	0	-1	0.25
cn_prsity6	0	-1	0.25

```
gr_strt4                0.0211893   -0.0222764   0.0108664
cn_rech5                 -0.09691           -1    0.225772
cn_strt6                0.0211893   -0.0222764   0.0108664
cn_ss8                          1           -1         0.5
gr_hk3                          1           -1         0.5
cn_sy6                   0.243038     -0.60206    0.211275
gr_prsity3                      0           -1        0.25
pp_vka0                         1           -1         0.5
gr_sy5                   0.243038     -0.60206    0.211275
pp_hk2                          1           -1         0.5
pp_vka2                         1           -1         0.5
pp_sy2                   0.243038     -0.60206    0.211275
pp_prsity2                      0           -1        0.25
strk                            2           -2           1
gr_vka3                         1           -1         0.5

[65 rows x 7 columns]
```

1.0.1 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 [4]:
```
par = pst.parameter_data
```

In [5]:
```
# 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[5]: 719

In [6]:
```
# 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[6]: 719

In [7]:
```
par.loc[par.pargp.apply(lambda x: "pp" in x),"pargp"].unique()
```

Out[7]:
```
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 [8]:
```
#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[8]:
```
719
```

In [9]:
```
adj_par = par.loc[par.partrans=="log",:]
adj_par.pargp.value_counts().sort_values()
```

Out[9]:
```
cn_rech5        1
cn_hk7          1
cn_sy7          1
cn_hk6          1
cn_sy8          1
cn_prsity7      1
cn_strt8        1
cn_rech4        1
cn_ss8          1
cn_vka6         1
cn_prsity8      1
cn_hk8          1
cn_strt7        1
cn_strt6        1
cn_vka7         1
cn_vka8         1
cn_ss6          1
cn_ss7          1
cn_prsity6      1
cn_sy6          1
flow            1
welflux         2
welflux_k02     6
drncond_k00    10
pp_prsity0     32
pp_vka0        32
pp_strt2       32
pp_rech0       32
pp_ss0         32
pp_rech1       32
pp_vka1        32
pp_prsity1     32
pp_hk1         32
pp_sy0         32
pp_ss1         32
pp_prsity2     32
pp_vka2        32
pp_sy1         32
```

```
pp_strt0       32
pp_strt1       32
pp_ss2         32
pp_hk0         32
pp_sy2         32
pp_hk2         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 [10]: 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[10]: 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 [11]: 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"))
```

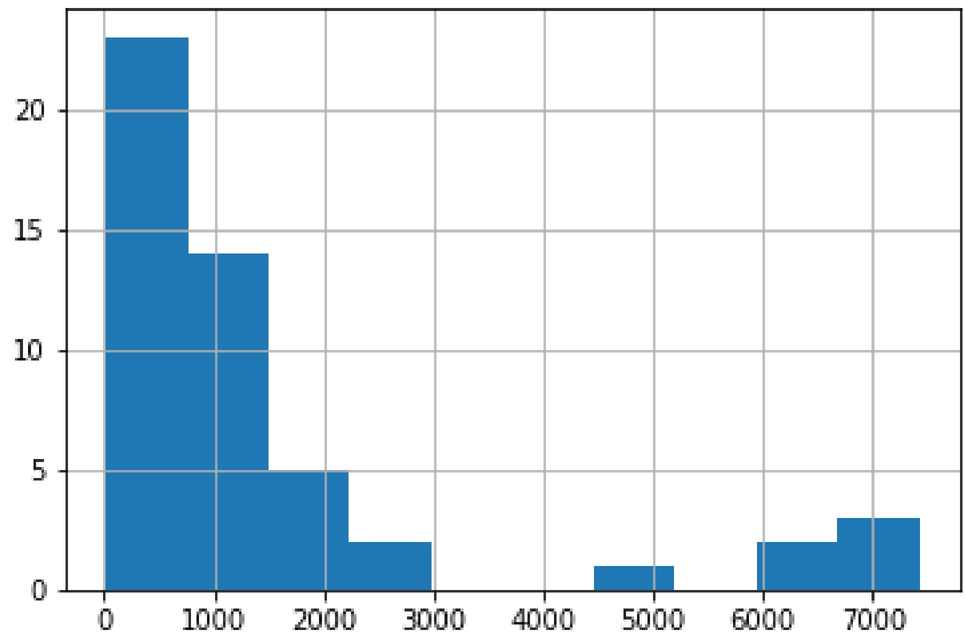
```
In [12]: #pyemu.os_utils.start_slaves(t_d,"pestpp-glm","freyberg_pp.pst",num_slaves=20,slave_r
         #                             master_dir=m_d)
```

```
In [13]: 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 [14]: ax = oe.phi_vector.hist()#bins=np.linspace(0,100,20))
         oe.phi_vector.sort_values().iloc[:20]
```

```
Out[14]: real_name
         1        16.417398
         23       40.379792
         21      136.184310
         10      188.214172
         26      229.596887
         8       280.037659
         16      302.087583
         41      303.432559
         12      332.762416
```

```
37    342.523602
30    346.262108
17    412.799856
0     444.770367
15    476.092295
5     479.962961
47    499.062079
46    531.175817
31    531.603828
33    561.768950
25    562.670514
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 [15]:
```
oe_pt = oe.loc[oe.phi_vector.sort_values().index[:20],:] #just take the 20 lowest phi
```

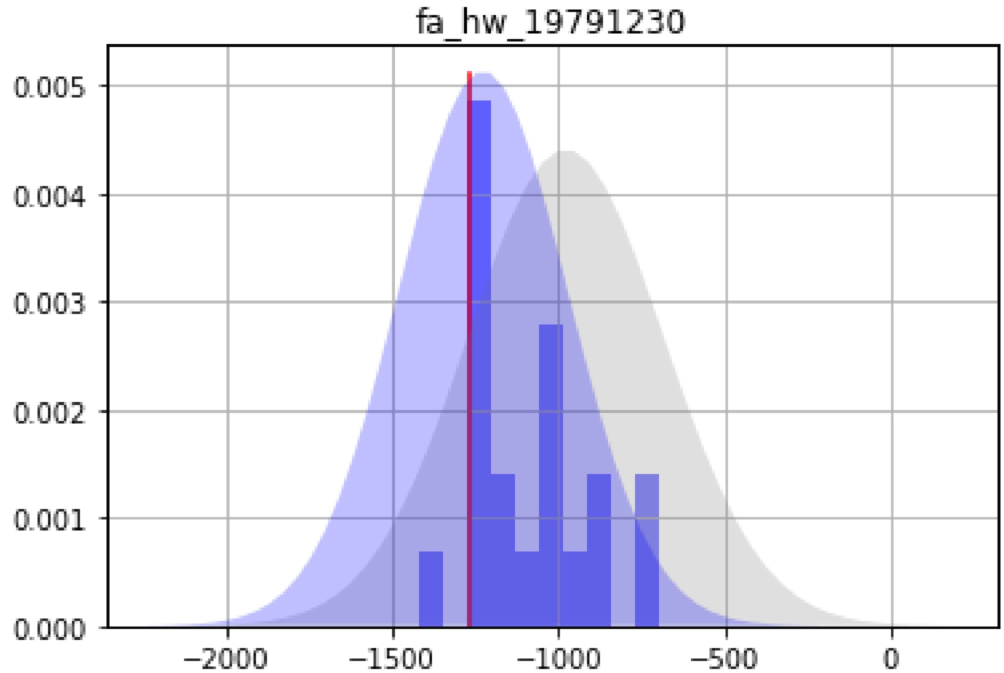
We can also load and plot the FOSM forecast results along side of the ensemble results:

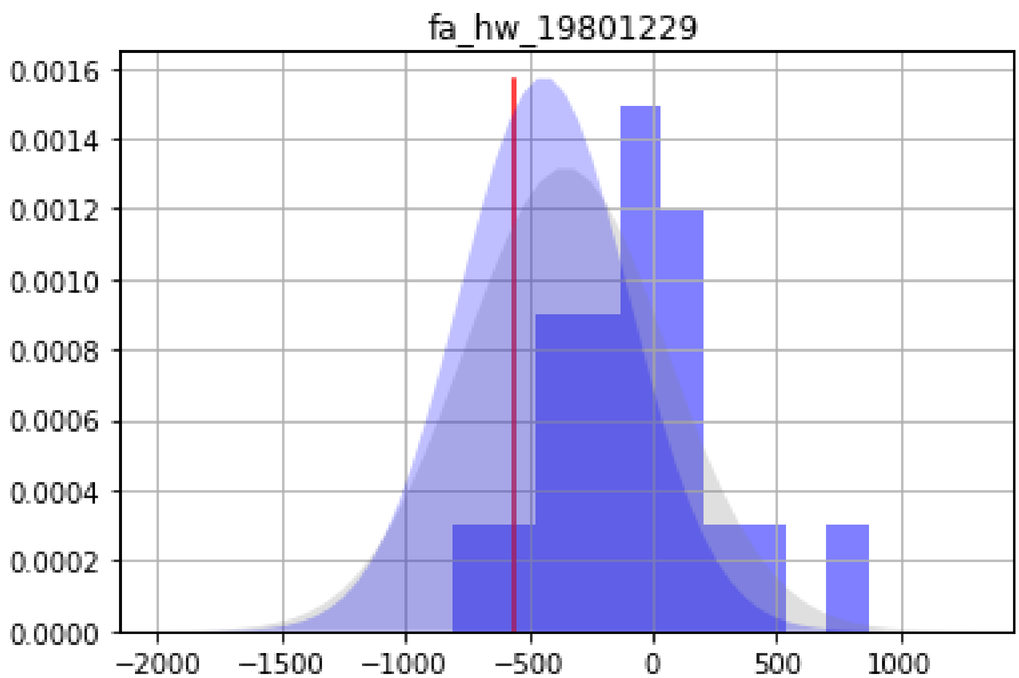
In [16]:
```
f_df = pd.read_csv(os.path.join(m_d,"freyberg_pp.pred.usum.csv"),index_col=0)
f_df.index = f_df.index.map(str.lower)
f_df
```

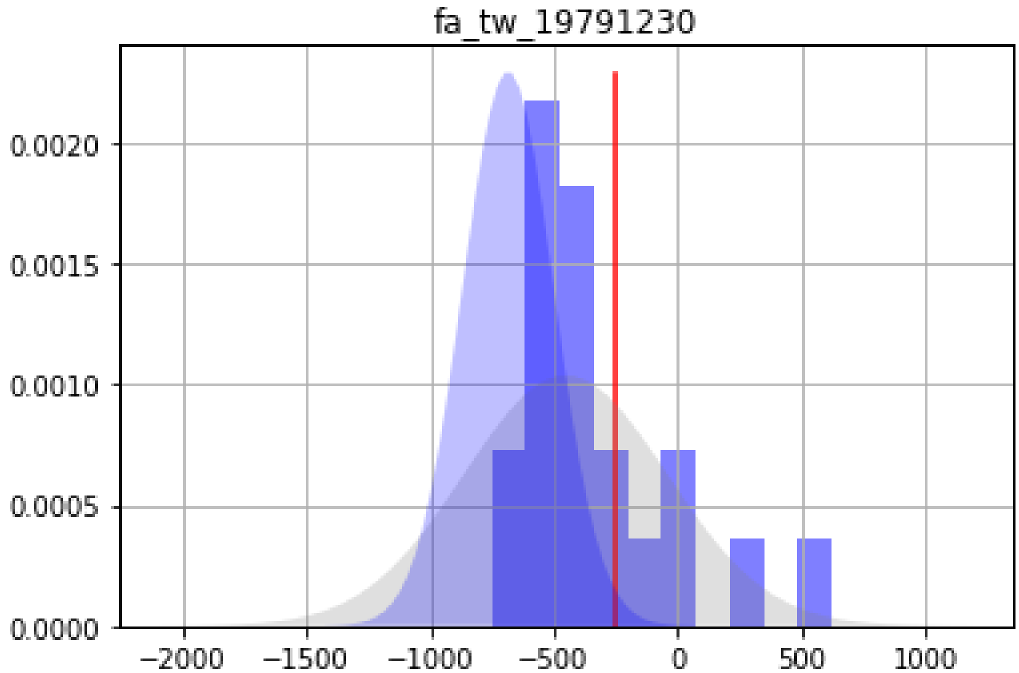
Out[16]:
```
                          prior_mean  prior_stdev  prior_lower_bound  \
name
```

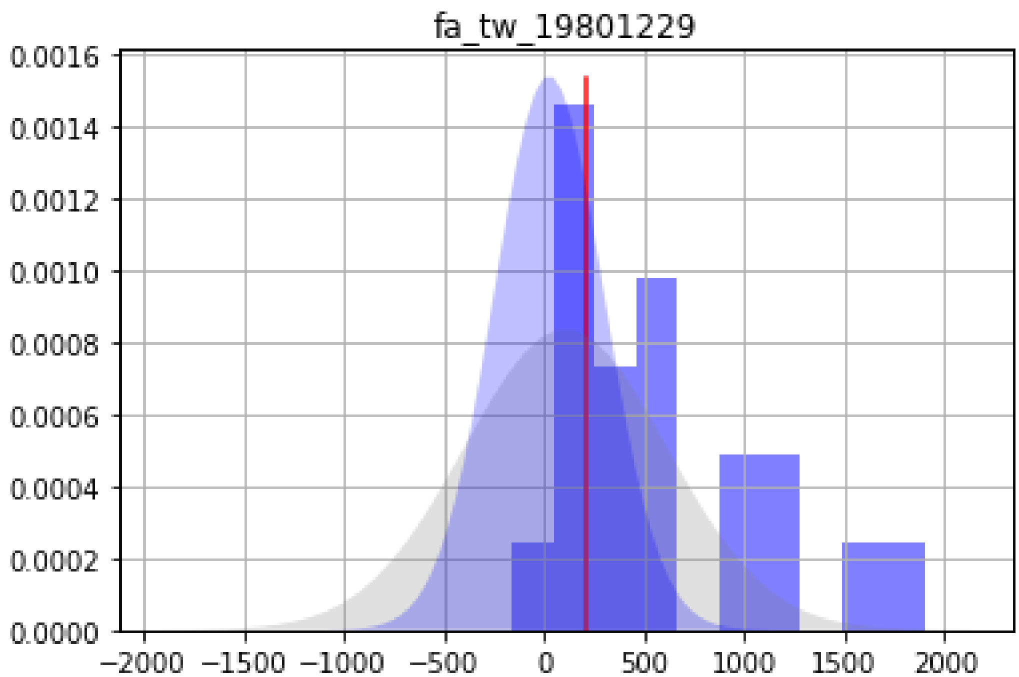
```
fa_hw_19791230       -977.2390    295.32800          -1567.8900
fa_hw_19801229       -351.2160    409.77000          -1170.7600
fa_tw_19791230       -453.0330    409.35100          -1271.7400
fa_tw_19801229        108.9600    506.73200           -904.5040
hds_00_013_002_000     39.6102      3.96314            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    704.75100           -501.8010

                    prior_upper_bound  post_mean  post_stdev  \
name
fa_hw_19791230               -386.5840 -1226.1600  253.662000
fa_hw_19801229                468.3240  -438.0650  342.835000
fa_tw_19791230                365.6690  -685.1120  185.061000
fa_tw_19801229               1122.4200    25.8356  275.087000
hds_00_013_002_000             47.5365    40.1357    0.528593
hds_00_013_002_001             46.4994    38.6689    0.821579
part_status                     2.0000     2.0000    0.000000
part_time                    2317.2000   864.5700  609.653000

                    post_lower_bound  post_upper_bound
name
fa_hw_19791230            -1733.4900         -718.8380
fa_hw_19801229            -1123.7400          247.6060
fa_tw_19791230            -1055.2300         -314.9900
fa_tw_19801229             -524.3380          576.0100
hds_00_013_002_000           39.0785           41.1929
hds_00_013_002_001           37.0257           40.3120
part_status                   2.0000            2.0000
part_time                  -354.7370         2083.8800
```

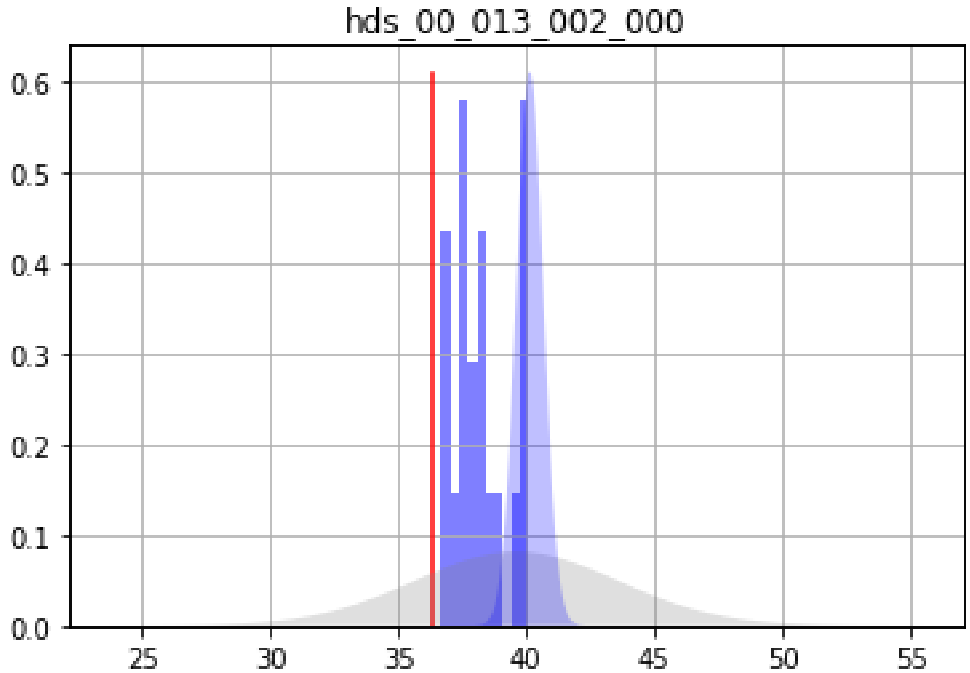
In [17]:
```
obs = pst.observation_data
fnames = pst.pestpp_options["forecasts"].split(",")
for forecast in fnames:
    ax = plt.subplot(111)
    oe_pt.loc[:,forecast].hist(ax=ax,color="b",alpha=0.5,normed=True)
    ax.plot([obs.loc[forecast,"obsval"],obs.loc[forecast,"obsval"]],ax.get_ylim(),"r"
    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()
```

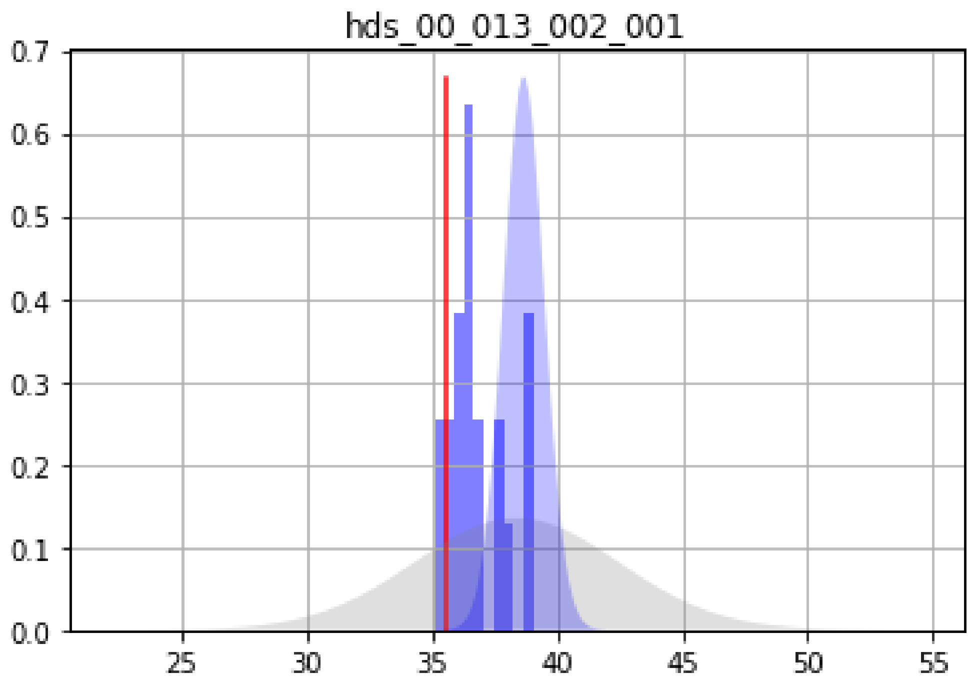

fa_hw_19791230
0.005
0.004
0.003
0.002
0.001
0.000
−2000
−1500
−1000
−500
0

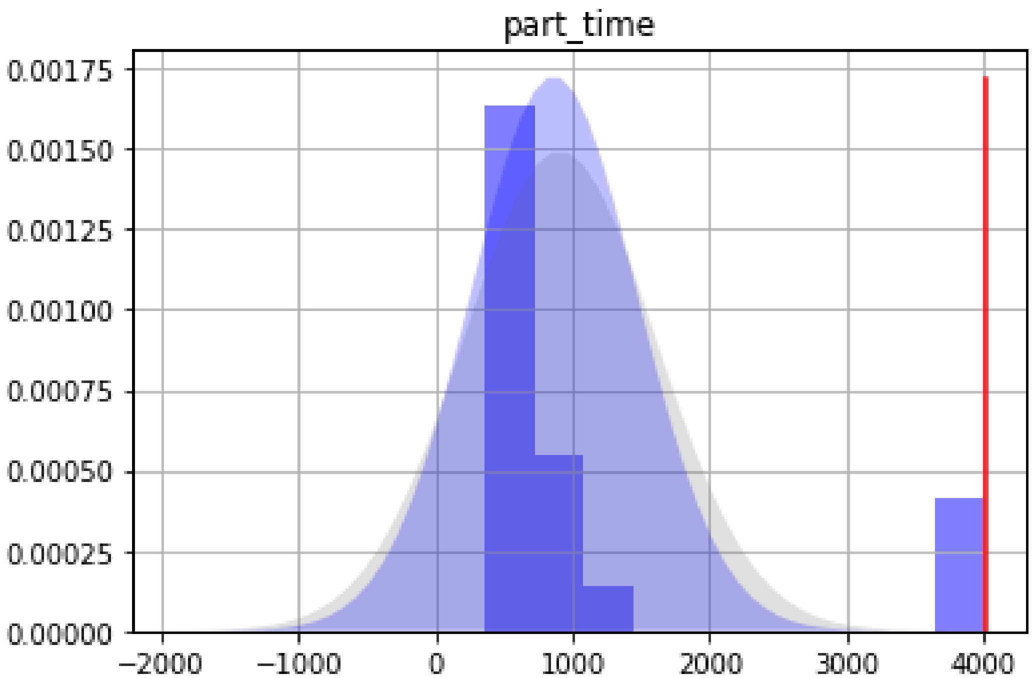

fa_hw_19801229
0.0016
0.0014
0.0012
0.0010
0.0008
0.0006
0.0004
0.0002
0.0000
−2000
−1500
−1000
−500
0
500
1000

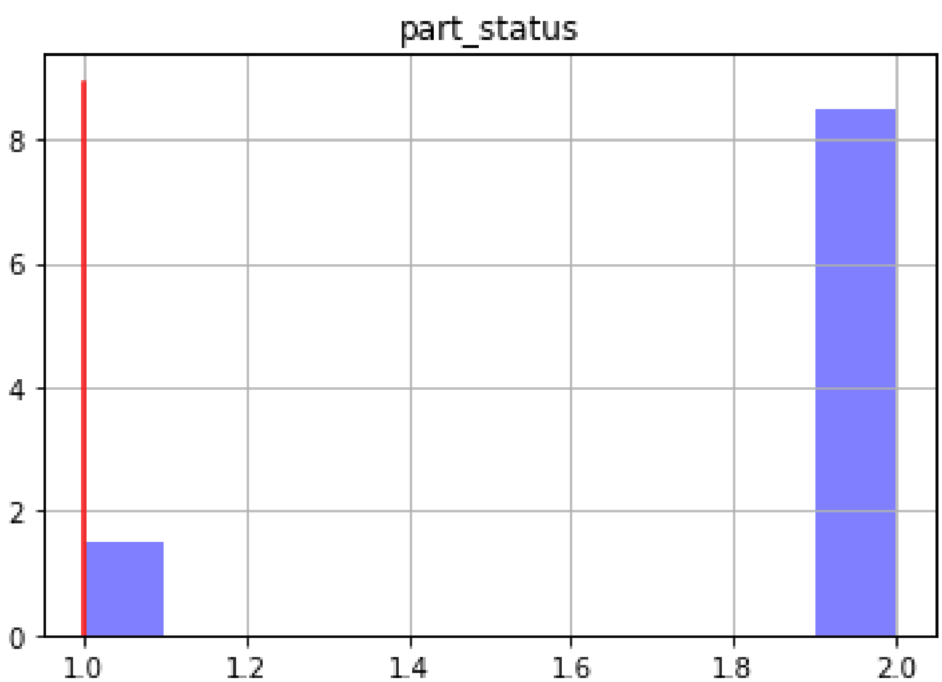

fa_tw_19791230
0.0020
0.0015
0.0010
0.0005
0.0000
−2000
−1500
−1000
−500
0
500
1000


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


part_time
0.00175
0.00150
0.00125
0.00100
0.00075
0.00050
0.00025
0.00000
−2000
−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

1.0.2 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 [18]: cov = pyemu.Cov.from_binary(os.path.join(t_d,"prior_cov.jcb"))
```

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

```
In [19]: pyemu.helpers.first_order_pearson_tikhonov(pst,cov)
```

```
getting CC matrix
processing
```

```
In [20]: pst.prior_information.head()
```

```
Out[20]:                                                        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 [21]: shutil.copy2(os.path.join(m_d,"freyberg_pp.jcb"),os.path.join(t_d,"restart_pp.jcb"))
```

```
Out[21]: 'template/restart_pp.jcb'
```

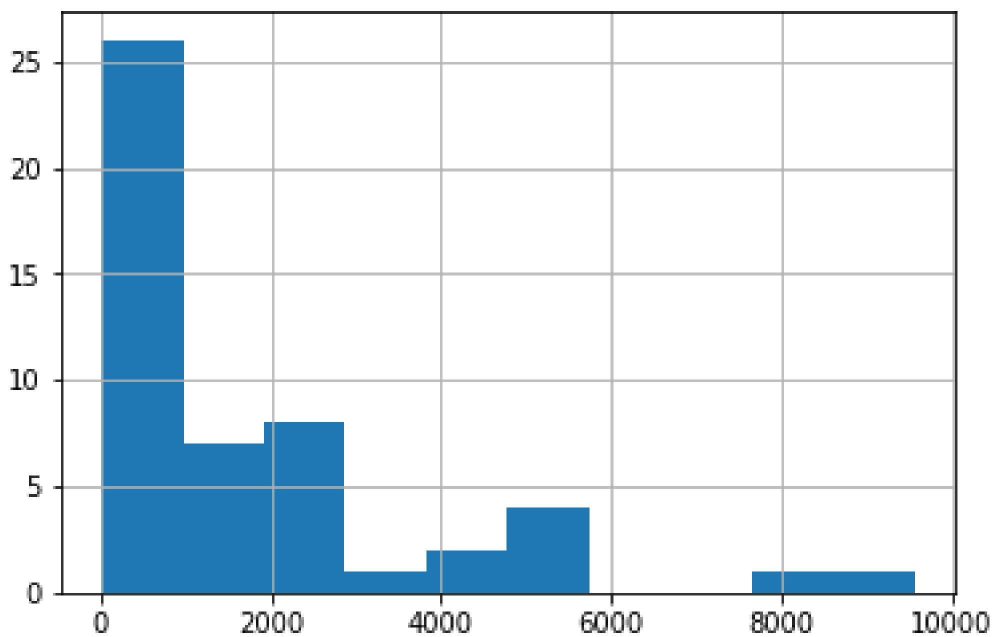
```
In [22]: pst.pestpp_options["base_jacobian"] = "restart_pp.jcb"
         pst.reg_data.phimlim = pst.nnz_obs
         pst.reg_data.phimaccept = pst.reg_data.phimlim * 1.1
         pst.write(os.path.join(t_d,"freyberg_pp.pst"))
```

```
In [23]: pyemu.os_utils.start_slaves(t_d,"pestpp-glm","freyberg_pp.pst",num_slaves=20,slave_ro
                                     master_dir=m_d)
```

```
In [24]: 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 [25]: ax = oe.phi_vector.hist()#bins=np.linspace(0,100,20))
         oe.phi_vector.sort_values().iloc[:20]
```

```
Out[25]: real_name
         36     15.065424
         5      32.066449
         15     37.431013
         23     48.812383
         8      51.256638
         37     58.762065
         33     58.770261
         45     66.702450
         48     72.439946
         7     119.140950
         35    135.031556
         39    142.732374
         21    164.359717
         19    172.289419
         10    189.037788
         34    215.624717
         17    268.322434
         49    302.529537
         1     380.312298
         6     382.312478
         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:

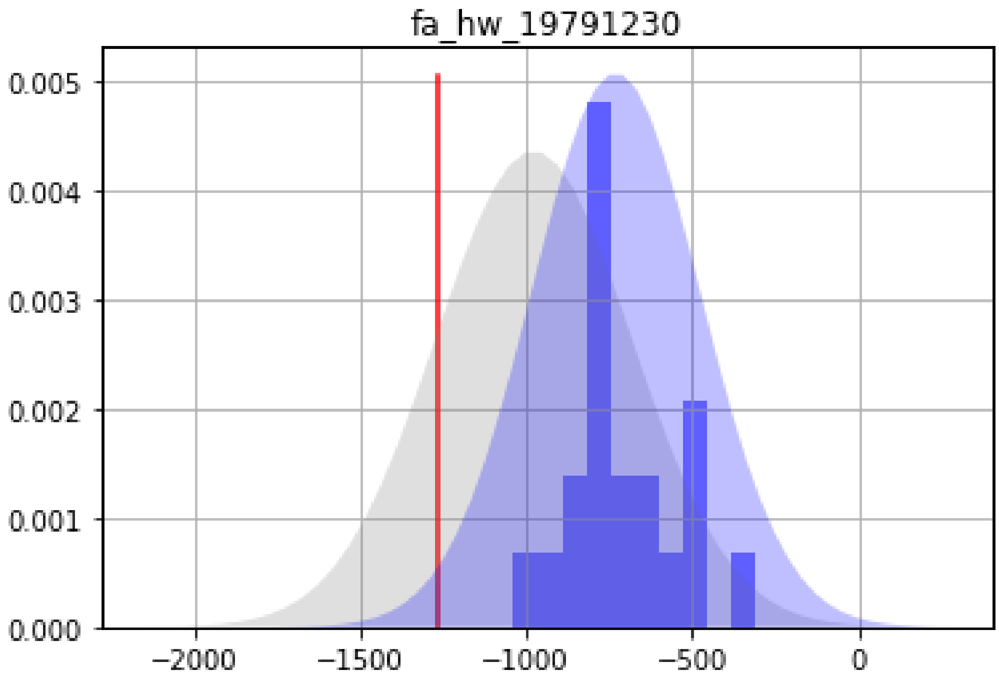
```
In [26]: oe_pt = oe.loc[oe.phi_vector.sort_values().index[:20],:]
```

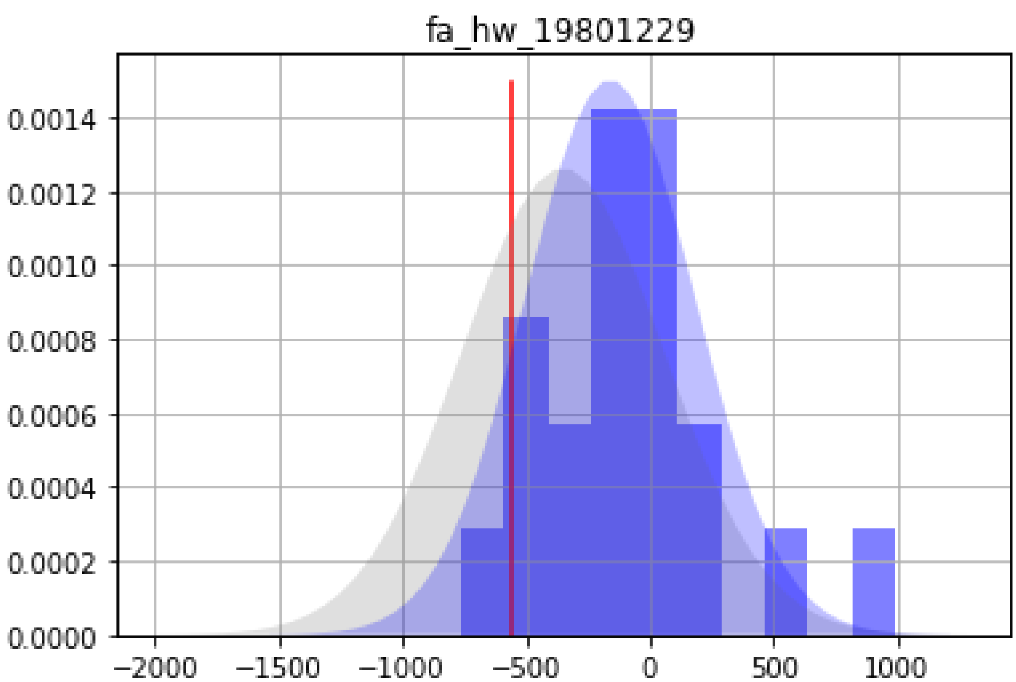
```
In [27]: f_df = pd.read_csv(os.path.join(m_d,"freyberg_pp.pred.usum.csv"),index_col=0)
         f_df.index = f_df.index.map(str.lower)
         f_df
```

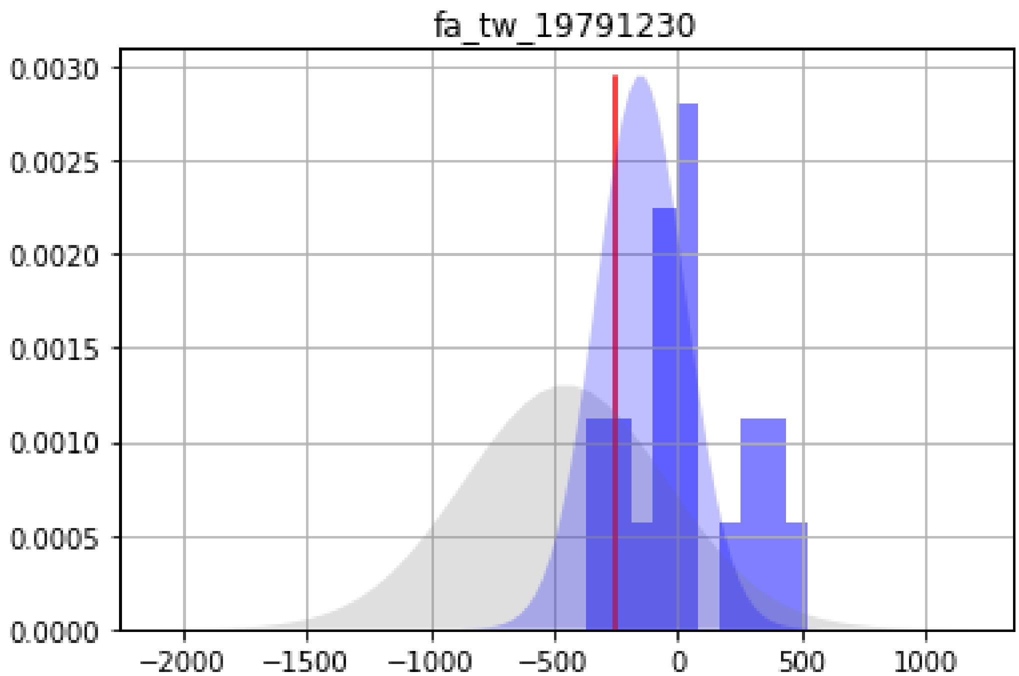
```
Out[27]:                    prior_mean  prior_stdev  prior_lower_bound  \
         name
         fa_hw_19791230       -977.2390    295.32800         -1567.8900
         fa_hw_19801229       -351.2160    409.77000         -1170.7600
         fa_tw_19791230       -453.0330    409.35100         -1271.7400
         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    704.75100          -501.8010

                            prior_upper_bound  post_mean  post_stdev  \
         name
         fa_hw_19791230              -386.5840  -729.6690  253.767000
         fa_hw_19801229               468.3240  -160.1280  344.320000
         fa_tw_19791230               365.6690  -149.8650  180.227000
         fa_tw_19801229              1122.4200   361.9180  272.345000
         hds_00_013_002_000            47.5365    36.9915    0.327097
         hds_00_013_002_001            46.4994    36.0961    0.710410
         part_status                    2.0000     1.0000    0.000000
         part_time                   2317.2000  4015.0000  604.279000

                            post_lower_bound  post_upper_bound
         name
         fa_hw_19791230             -1237.2000         -222.1350
         fa_hw_19801229              -848.7680          528.5130
         fa_tw_19791230              -510.3190          210.5890
         fa_tw_19801229              -182.7730          906.6090
         hds_00_013_002_000            36.3373           37.6457
         hds_00_013_002_001            34.6753           37.5170
         part_status                    1.0000            1.0000
         part_time                   2806.4400         5223.5600
```

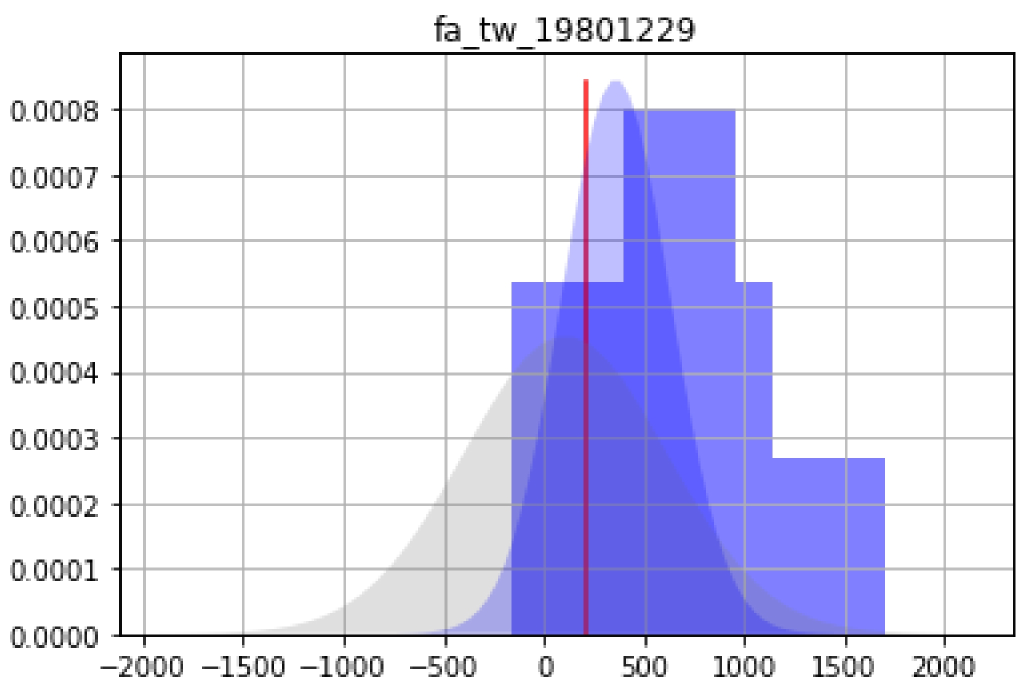
```
In [28]: obs = pst.observation_data
         fnames = pst.pestpp_options["forecasts"].split(",")
         for forecast in fnames:
             ax = plt.subplot(111)
             oe_pt.loc[:,forecast].hist(ax=ax,color="b",alpha=0.5,normed=True)
             ax.plot([obs.loc[forecast,"obsval"],obs.loc[forecast,"obsval"]],ax.get_ylim(),"r"
             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)
```

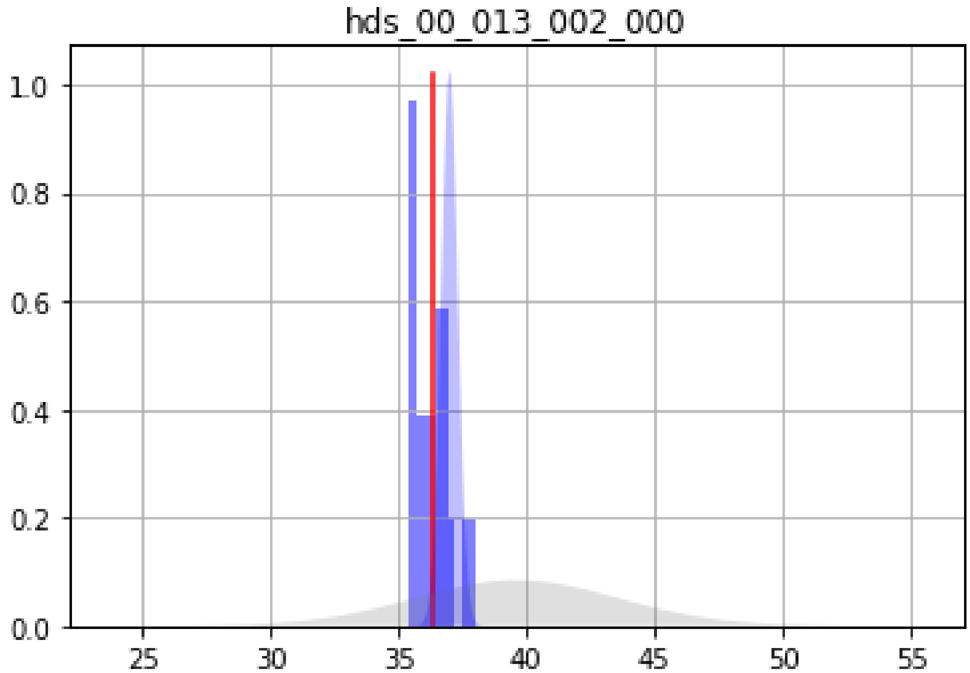
```
axt.set_ylim(0,axt.get_ylim()[1])
axt.set_yticks([])
ax.set_title(forecast)
plt.show()
```

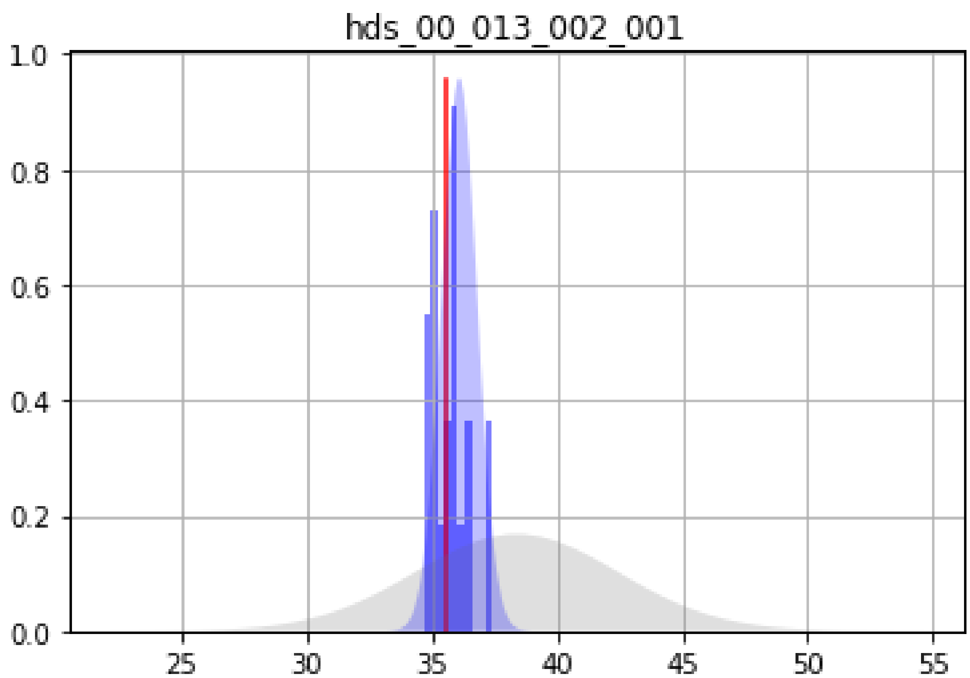


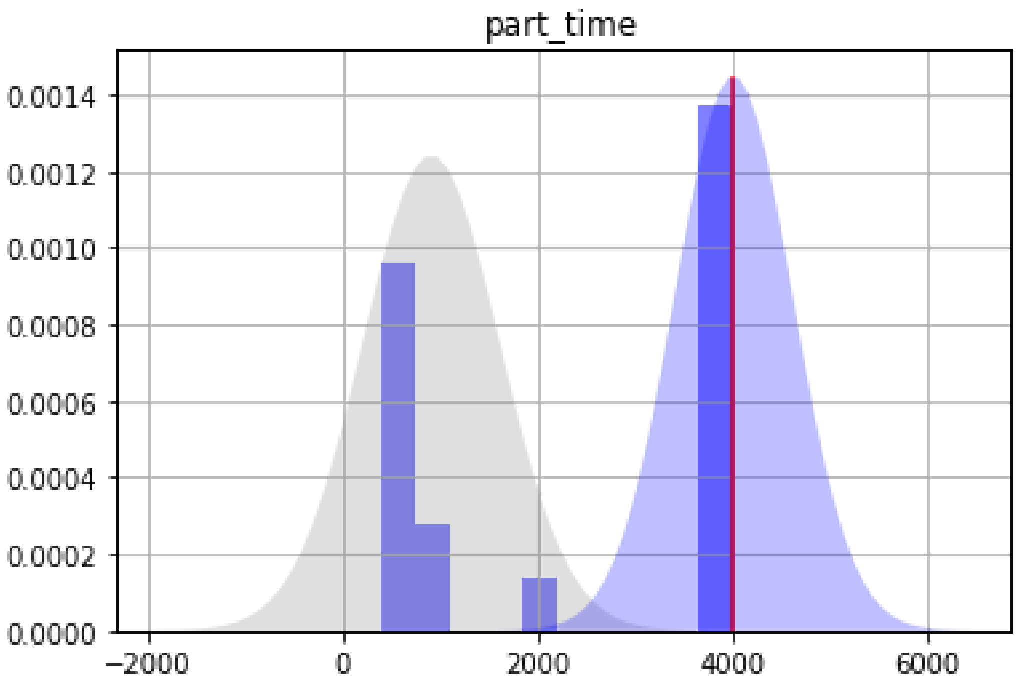


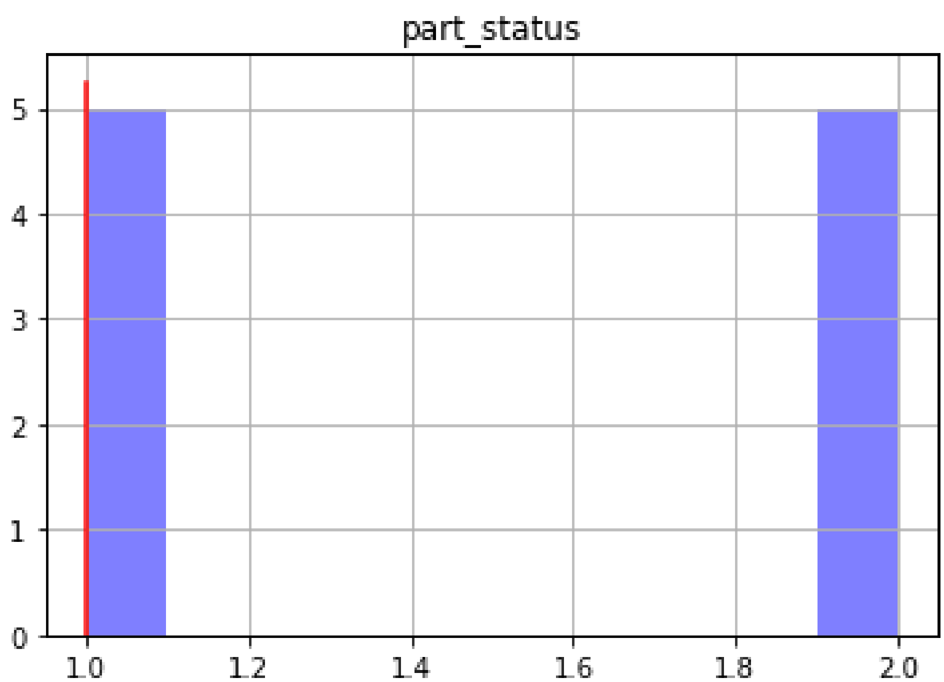

fa_tw_19791230
0.0030
0.0025
0.0020
0.0015
0.0010
0.0005
0.0000
−2000
−1500
−1000
−500
0
500
1000


fa_tw_19801229
0.0008
0.0007
0.0006
0.0005
0.0004
0.0003
0.0002
0.0001
0.0000
−2000
−1500
−1000
−500
0
500
1000
1500
2000


hds_00_013_002_000
1.0
0.8
0.6
0.4
0.2
0.0
25
30
35
40
45
50
55


hds_00_013_002_001
1.0
0.8
0.6
0.4
0.2
0.0
25
30
35
40
45
50
55


part_time
0.0014
0.0012
0.0010
0.0008
0.0006
0.0004
0.0002
0.0000
−2000
0
2000
4000
6000


part_status
5
4
3
2
1
0
1.0
1.2
1.4
1.6
1.8
2.0