pestpp-glm

May 3, 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  \
        gr_sy4            gr_sy4       log    705                  0
        gr_prsity4    gr_prsity4       log    705                  0
        cn_strt6        cn_strt6       log      1                  0
        strk                strk       log     40                  0
        cn_ss8            cn_ss8       log      1                  0
        gr_rech3        gr_rech3       log    705                  0
        gr_sy5            gr_sy5       log    705                  0
        pp_rech1        pp_rech1       log     32                  0
        gr_sy3            gr_sy3       log    705                  0
        cn_sy8            cn_sy8       log      1                  0
        gr_vka3          gr_vka3       log    705                  0
        pp_hk1            pp_hk1       log     32                  0
        cn_vka8          cn_vka8       log      1                  0
```

cn_hk7	cn_hk7	log	1	0
pp_prsity1	pp_prsity1	log	32	0
pp_ss0	pp_ss0	log	32	0
pp_strt0	pp_strt0	log	32	0
pp_hk0	pp_hk0	log	32	0
pp_ss1	pp_ss1	log	32	0
pp_hk2	pp_hk2	log	32	0
flow	flow	log	1	0
pp_ss2	pp_ss2	log	32	0
pp_rech0	pp_rech0	log	32	0
pp_prsity0	pp_prsity0	log	32	0
gr_strt4	gr_strt4	log	705	0
gr_strt5	gr_strt5	log	705	0
pp_prsity2	pp_prsity2	log	32	0
cn_rech5	cn_rech5	log	1	-0.39794
gr_rech2	gr_rech2	log	705	0
gr_hk3	gr_hk3	log	705	0
...	...	...	...	...
gr_ss5	gr_ss5	log	705	0
cn_strt8	cn_strt8	log	1	0
pp_strt2	pp_strt2	log	32	0
pp_vka0	pp_vka0	log	32	0
cn_ss6	cn_ss6	log	1	0
cn_hk8	cn_hk8	log	1	0
welflux_k02	welflux_k02	log	6	0
gr_strt3	gr_strt3	log	705	0
cn_vka7	cn_vka7	log	1	0
gr_vka4	gr_vka4	log	705	0
cn_prsity6	cn_prsity6	log	1	0
cn_prsity7	cn_prsity7	log	1	0
cn_sy6	cn_sy6	log	1	0
pp_sy0	pp_sy0	log	32	0
gr_ss3	gr_ss3	log	705	0
cn_hk6	cn_hk6	log	1	0
cn_sy7	cn_sy7	log	1	0
drncond_k00	drncond_k00	log	10	0
gr_hk5	gr_hk5	log	705	0
pp_sy1	pp_sy1	log	32	0
cn_prsity8	cn_prsity8	log	1	0
gr_prsity3	gr_prsity3	log	705	0
welflux	welflux	log	2	0 to 0.176091
gr_hk4	gr_hk4	log	705	0
gr_vka5	gr_vka5	log	705	0
cn_ss7	cn_ss7	log	1	0
pp_vka1	pp_vka1	log	32	0
pp_strt1	pp_strt1	log	32	0
cn_rech4	cn_rech4	log	1	0
gr_prsity5	gr_prsity5	log	705	0

	upper bound	lower bound	standard deviation
gr_sy4	0.243038	-0.60206	0.211275
gr_prsity4	0	-1	0.25
cn_strt6	0.0211893	-0.0222764	0.0108664
strk	2	-2	1
cn_ss8	1	-1	0.5
gr_rech3	0.0413927	-0.0457575	0.0217875
gr_sy5	0.243038	-0.60206	0.211275
pp_rech1	0.0413927	-0.0457575	0.0217875
gr_sy3	0.243038	-0.60206	0.211275
cn_sy8	0.243038	-0.60206	0.211275
gr_vka3	1	-1	0.5
pp_hk1	1	-1	0.5
cn_vka8	1	-1	0.5
cn_hk7	1	-1	0.5
pp_prsity1	0	-1	0.25
pp_ss0	1	-1	0.5
pp_strt0	0.0211893	-0.0222764	0.0108664
pp_hk0	1	-1	0.5
pp_ss1	1	-1	0.5
pp_hk2	1	-1	0.5
flow	0.09691	-0.124939	0.0554622
pp_ss2	1	-1	0.5
pp_rech0	0.0413927	-0.0457575	0.0217875
pp_prsity0	0	-1	0.25
gr_strt4	0.0211893	-0.0222764	0.0108664
gr_strt5	0.0211893	-0.0222764	0.0108664
pp_prsity2	0	-1	0.25
cn_rech5	-0.09691	-1	0.225772
gr_rech2	0.0413927	-0.0457575	0.0217875
gr_hk3	1	-1	0.5
...	...	...	...
gr_ss5	1	-1	0.5
cn_strt8	0.0211893	-0.0222764	0.0108664
pp_strt2	0.0211893	-0.0222764	0.0108664
pp_vka0	1	-1	0.5
cn_ss6	1	-1	0.5
cn_hk8	1	-1	0.5
welflux_k02	1	-1	0.5
gr_strt3	0.0211893	-0.0222764	0.0108664
cn_vka7	1	-1	0.5
gr_vka4	1	-1	0.5
cn_prsity6	0	-1	0.25
cn_prsity7	0	-1	0.25
cn_sy6	0.243038	-0.60206	0.211275
pp_sy0	0.243038	-0.60206	0.211275
gr_ss3	1	-1	0.5

```
cn_hk6                            1              -1                   0.5
cn_sy7                     0.243038        -0.60206              0.211275
drncond_k00                       1              -1                   0.5
gr_hk5                            1              -1                   0.5
pp_sy1                     0.243038        -0.60206              0.211275
cn_prsity8                        0              -1                  0.25
gr_prsity3                        0              -1                  0.25
welflux      0.176091 to 0.30103  -0.30103 to     0  0.0752575 to 0.11928
gr_hk4                            1              -1                   0.5
gr_vka5                           1              -1                   0.5
cn_ss7                            1              -1                   0.5
pp_vka1                           1              -1                   0.5
pp_strt1                  0.0211893      -0.0222764             0.0108664
cn_rech4                  0.0791812        -0.09691             0.0440228
gr_prsity5                        0              -1                  0.25

[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_strt6        1
cn_rech4        1
cn_hk7          1
cn_sy8          1
cn_sy7          1
cn_ss8          1
cn_vka8         1
cn_vka6         1
flow            1
cn_rech5        1
cn_vka7         1
cn_strt7        1
cn_strt8        1
cn_hk8          1
cn_ss6          1
cn_prsity7      1
cn_sy6          1
cn_hk6          1
cn_prsity6      1
cn_prsity8      1
cn_ss7          1
welflux         2
welflux_k02     6
drncond_k00    10
pp_strt0       32
pp_rech0       32
pp_hk0         32
pp_sy2         32
pp_vka2        32
pp_ss0         32
pp_vka0        32
pp_sy0         32
pp_prsity2     32
pp_hk2         32
pp_strt2       32
pp_ss1         32
pp_ss2         32
pp_prsity1     32
```

```
pp_rech1       32
pp_sy1         32
pp_prsity0     32
pp_vka1        32
pp_strt1       32
pp_hk1         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"))
```

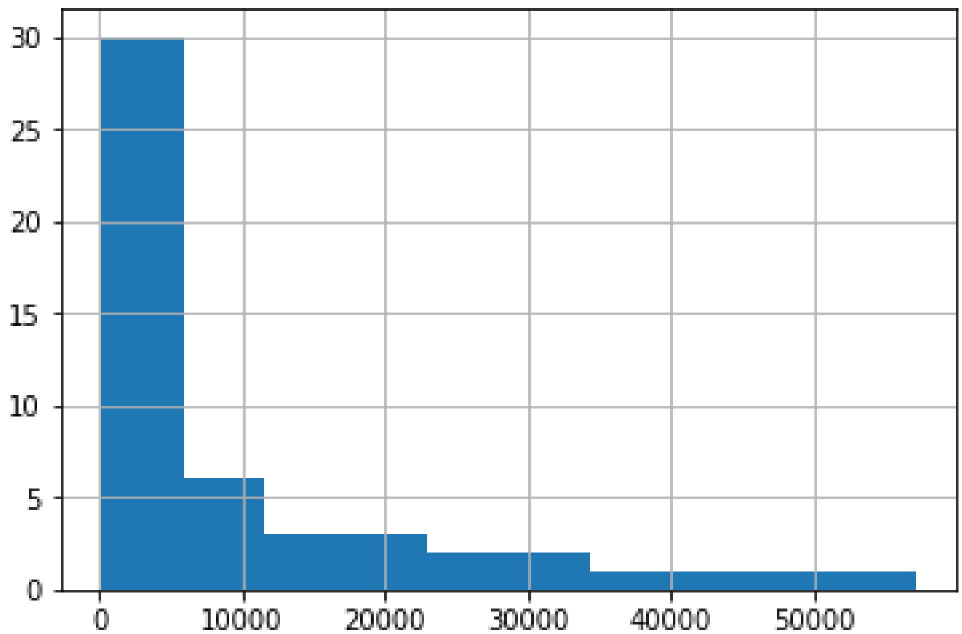
```
In [12]: #pyemu.os_utils.start_slaves(t_d,"pestpp-glm","freyberg_pp.pst",num_slaves=20,slave_r
         #                            master_dir=m_d)
```

```
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
         7       181.835972
         23      307.875113
         25      461.423208
         21      508.389022
         44      531.916245
         19      710.543355
         6       722.088590
         45      882.682950
         8       947.056165
```

```
9      1055.322092
24     1124.430746
33     1472.494248
11     1591.305572
17     1832.739231
34     2077.463682
30     2169.778154
27     2339.569383
46     2498.302887
49     2611.632003
41     2715.695479
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
```

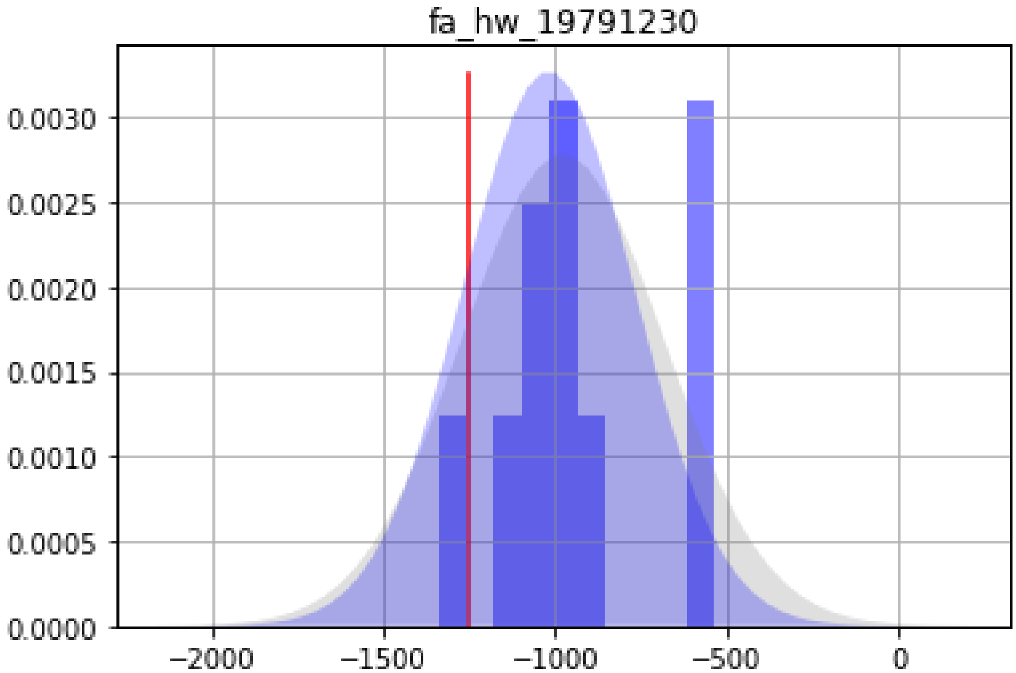
We can also load and plot the FOSM forecast results along side of the ensemble results:

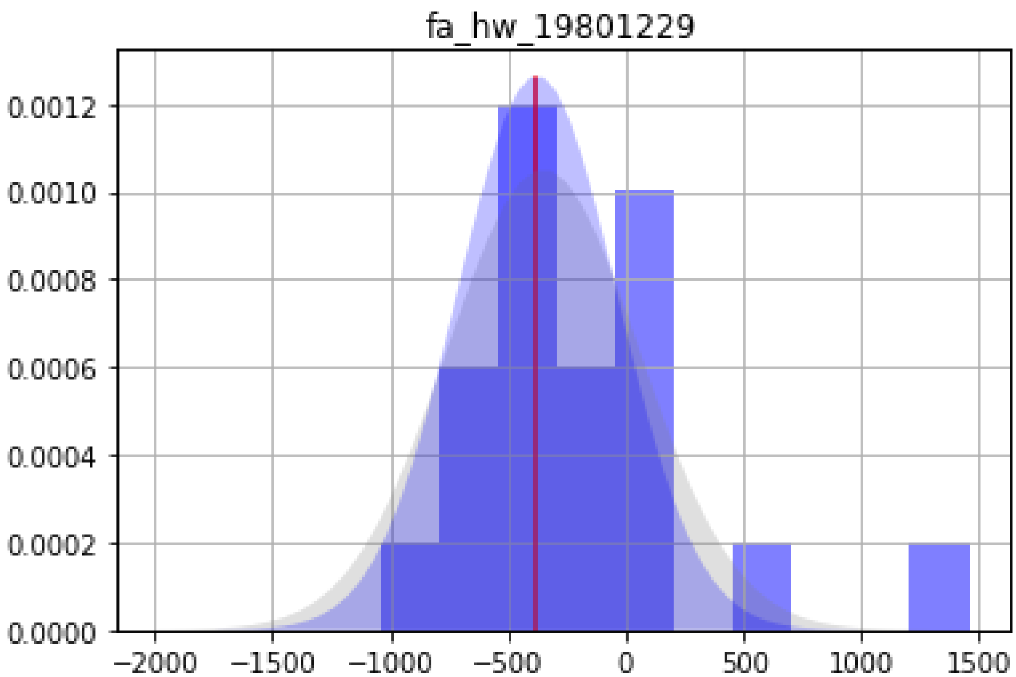
```
In [16]: f_df = pd.read_csv(os.path.join(m_d,"freyberg_pp.pred.usum.csv"),index_col=0)
         f_df.index = f_df.index.map(str.lower)
         f_df
```

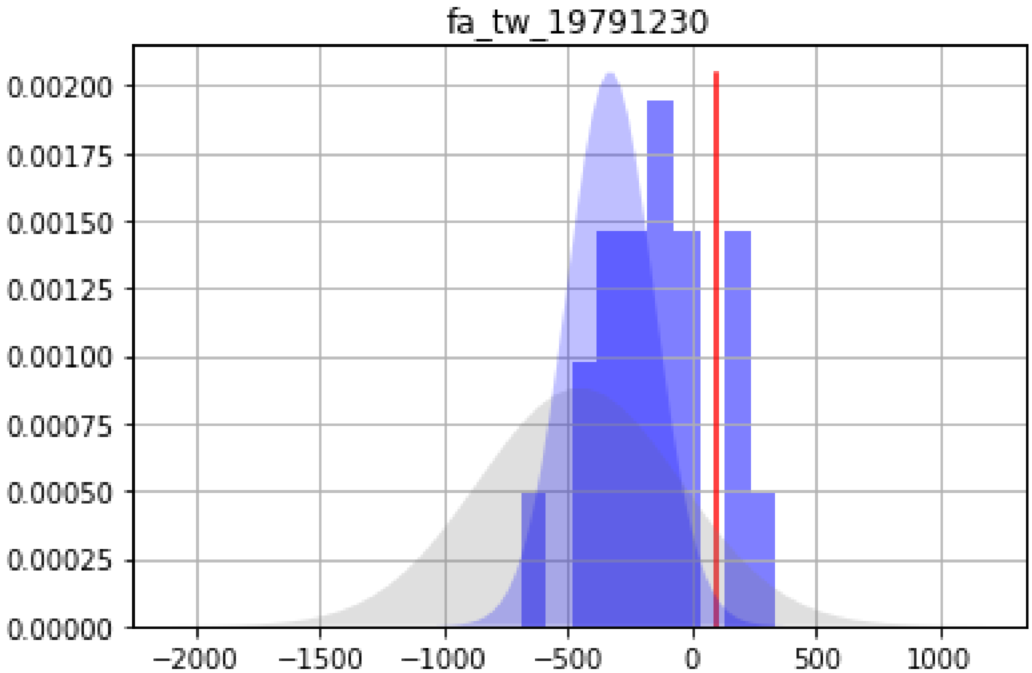
```
Out[16]:                          prior_mean  prior_stdev  prior_lower_bound  \
         name
```

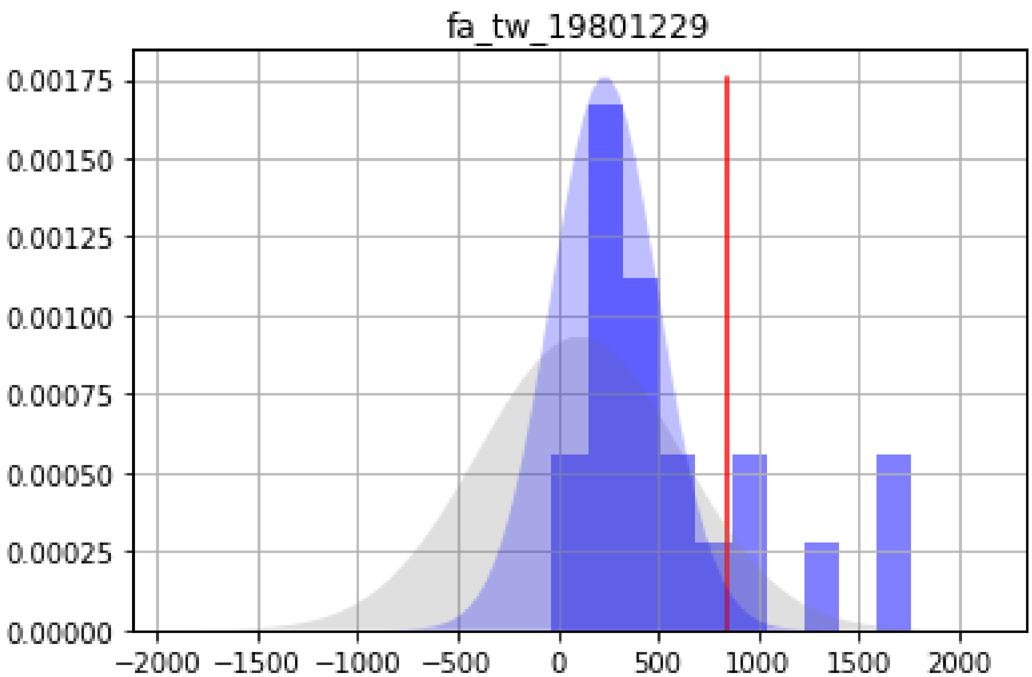
```
fa_hw_19791230       -977.2390    295.32800         -1567.8900
fa_hw_19801229       -351.2160    409.77000         -1170.7600
fa_tw_19791230       -453.0330    409.35100         -1271.7400
fa_tw_19801229        108.9600    506.73200          -904.5040
hds_00_013_002_000     39.6102      3.96314            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 -1019.0700  251.100000
fa_hw_19801229                468.3240  -377.4560  340.542000
fa_tw_19791230                365.6690  -329.7400  175.584000
fa_tw_19801229               1122.4200   234.8450  268.440000
hds_00_013_002_000             47.5365    39.1429    0.295060
hds_00_013_002_001             46.4994    37.8161    0.696415
part_status                     2.0000     2.0000    0.000000
part_time                    2317.2000  1348.2500  603.218000

                    post_lower_bound  post_upper_bound
name
fa_hw_19791230             -1521.2700         -516.8720
fa_hw_19801229             -1058.5400          303.6270
fa_tw_19791230              -680.9080           21.4276
fa_tw_19801229              -302.0350          771.7250
hds_00_013_002_000            38.5528           39.7330
hds_00_013_002_001            36.4233           39.2090
part_status                    2.0000            2.0000
part_time                    141.8160         2554.6900
```

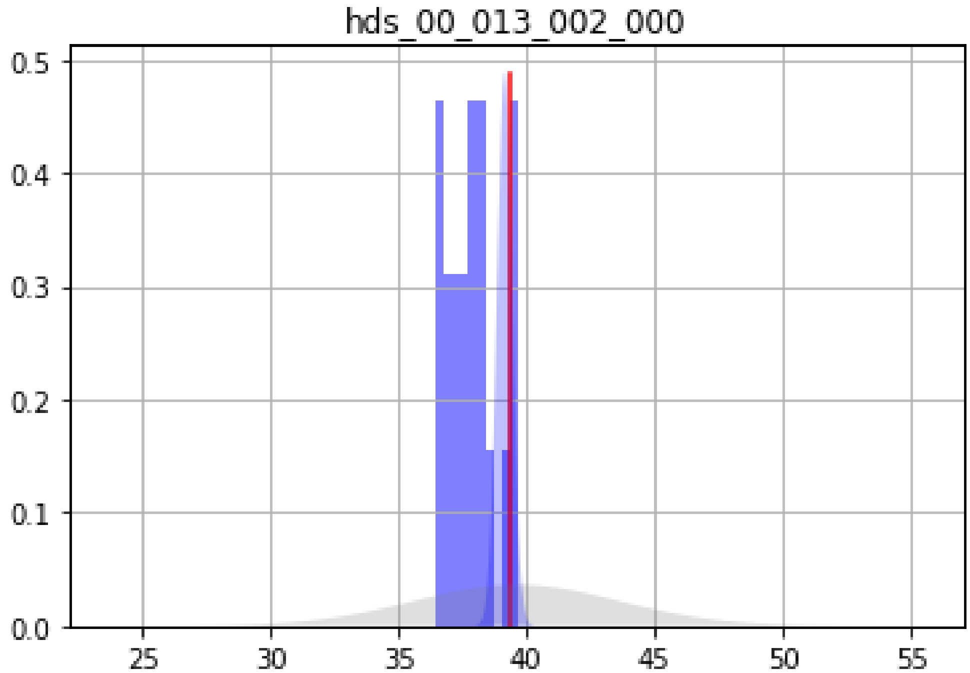
In [17]:
```
obs = pst.observation_data
fnames = pst.pestpp_options["forecasts"].split(",")
for forecast in fnames:
    ax = plt.subplot(111)
    oe_pt.loc[:,forecast].hist(ax=ax,color="b",alpha=0.5,normed=True)
    ax.plot([obs.loc[forecast,"obsval"],obs.loc[forecast,"obsval"]],ax.get_ylim(),"r"
  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

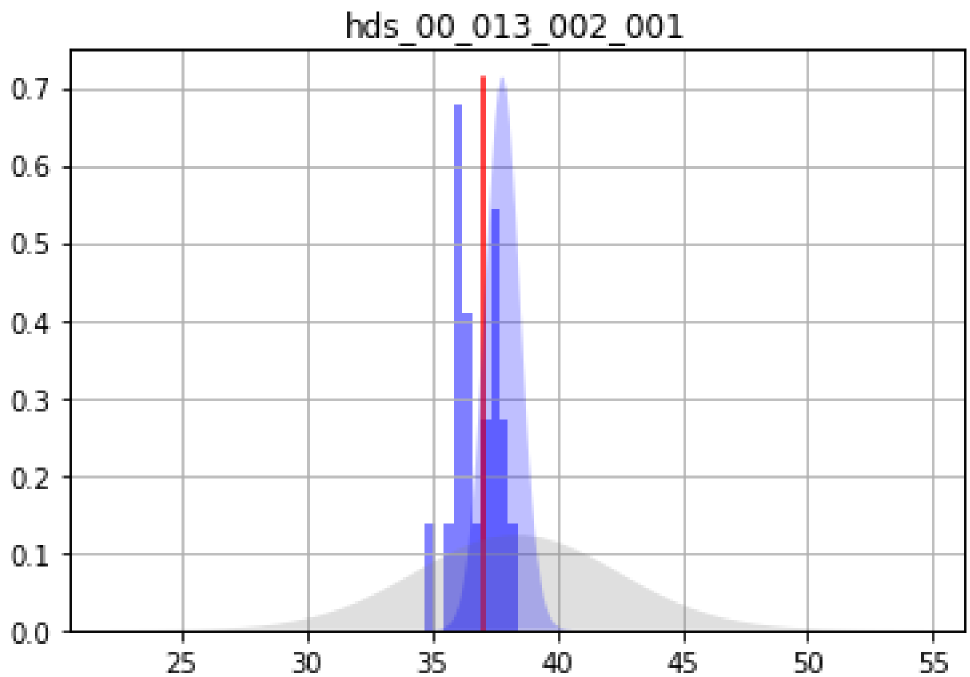

fa_hw_19791230
0.0030
0.0025
0.0020
0.0015
0.0010
0.0005
0.0000
−2000
−1500
−1000
−500
0

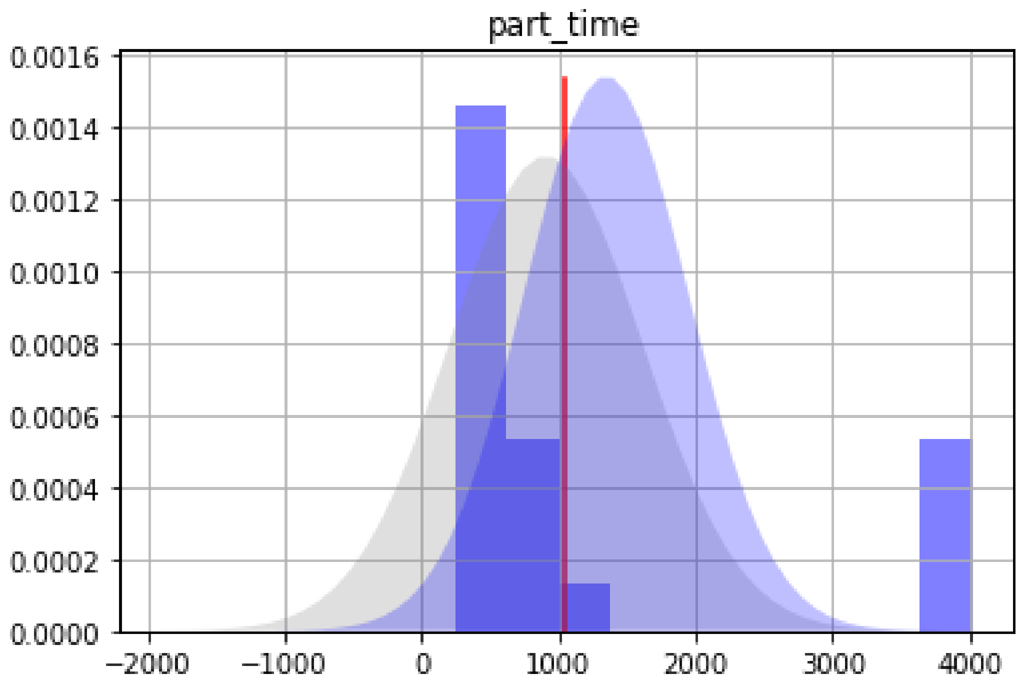

fa_hw_19801229
0.0012
0.0010
0.0008
0.0006
0.0004
0.0002
0.0000
−2000
−1500
−1000
−500
0
500
1000
1500

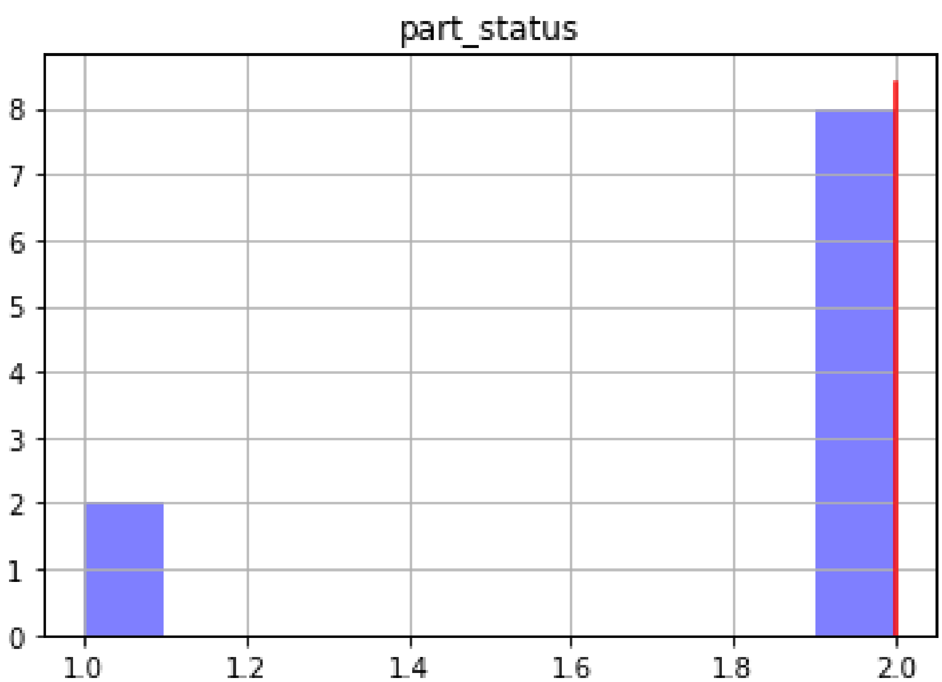

fa_tw_19791230
0.00200
0.00175
0.00150
0.00125
0.00100
0.00075
0.00050
0.00025
0.00000
−2000
−1500
−1000
−500
0
500
1000


fa_tw_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


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


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


part_time
0.0016
0.0014
0.0012
0.0010
0.0008
0.0006
0.0004
0.0002
0.0000
−2000
−1000
0
1000
2000
3000
4000


part_status
8
7
6
5
4
3
2
1
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'
```

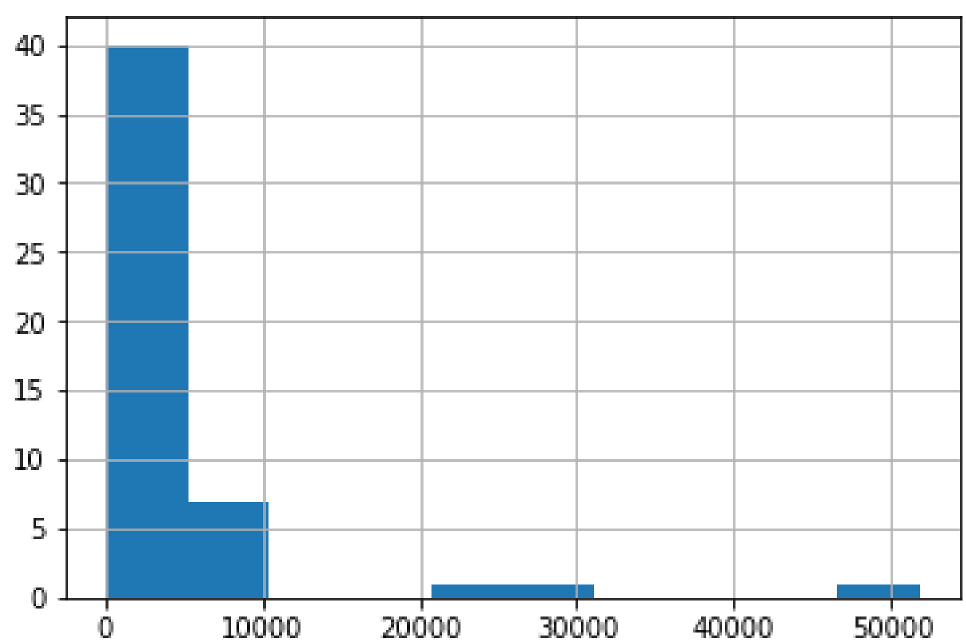
```
In [22]: pst.pestpp_options["base_jacobian"] = "restart_pp.jcb"
         pst.reg_data.phimlim = pst.nnz_obs
         pst.reg_data.phimaccept = pst.reg_data.phimlim * 1.1
         pst.write(os.path.join(t_d,"freyberg_pp.pst"))
```

```
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
26       93.513954
6       217.293403
23      226.100858
33      232.205306
22      308.050204
25      347.906426
45      429.314289
32      482.540726
44      557.405461
46      570.260765
47      595.014360
40      623.244712
4       638.025129
17      671.096086
15      676.631334
11      781.666502
5       834.788458
48     1223.998840
12     1249.309590
37     1631.682572
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:

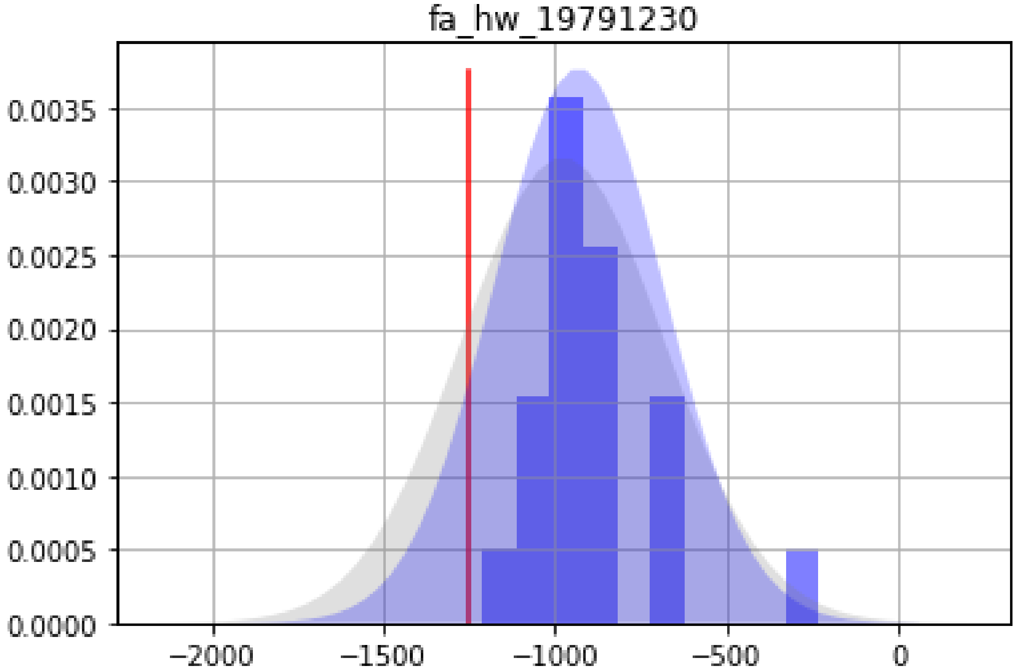
```
In [26]: oe_pt = oe.loc[oe.phi_vector.sort_values().index[:20],:]
```

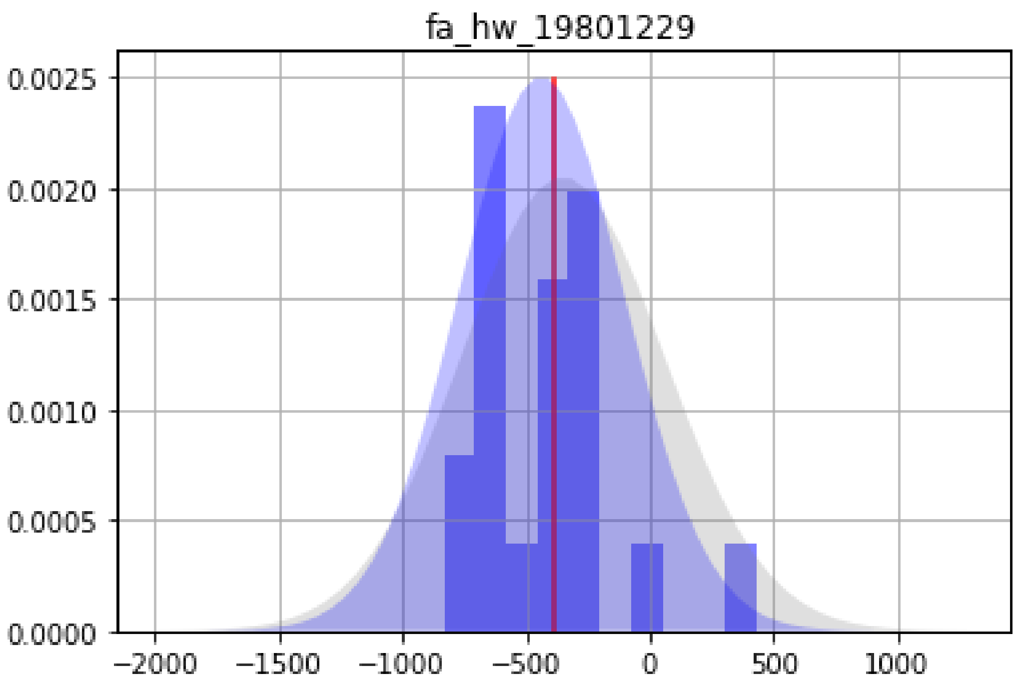
In [27]:
```
f_df = pd.read_csv(os.path.join(m_d,"freyberg_pp.pred.usum.csv"),index_col=0)
f_df.index = f_df.index.map(str.lower)
f_df
```

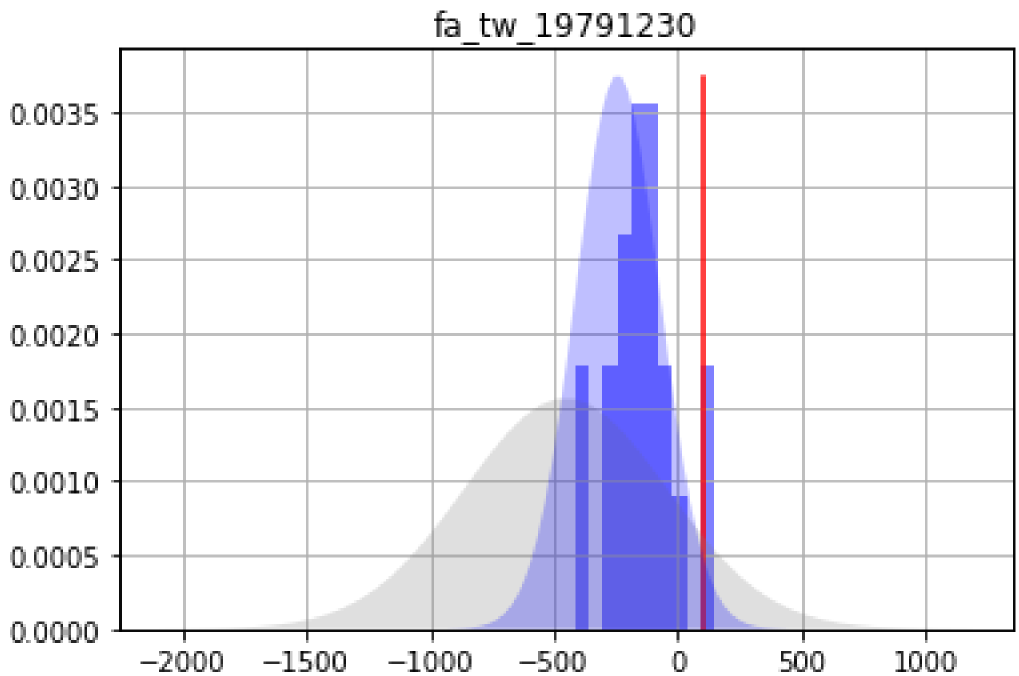
Out[27]:
```
                     prior_mean  prior_stdev  prior_lower_bound  \
name
fa_hw_19791230        -977.2390    295.32800         -1567.8900
fa_hw_19801229        -351.2160    409.77000         -1170.7600
fa_tw_19791230        -453.0330    409.35100         -1271.7400
fa_tw_19801229         108.9600    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  -931.1650  247.835000
fa_hw_19801229                468.3240  -438.0700  335.549000
fa_tw_19791230                365.6690  -242.9430  170.577000
fa_tw_19801229               1122.4200   272.6840  263.671000
hds_00_013_002_000             47.5365    39.1357    0.273990
hds_00_013_002_001             46.4994    38.0574    0.687833
part_status                     2.0000     2.0000    0.000000
part_time                    2317.2000  1060.4200  601.307000

                     post_lower_bound  post_upper_bound
name
fa_hw_19791230             -1426.8300         -435.4950
fa_hw_19801229             -1109.1700          233.0270
fa_tw_19791230              -584.0980           98.2112
fa_tw_19801229              -254.6580          800.0260
hds_00_013_002_000            38.5877           39.6836
hds_00_013_002_001            36.6818           39.4331
part_status                    2.0000            2.0000
part_time                   -142.1900         2263.0400
```

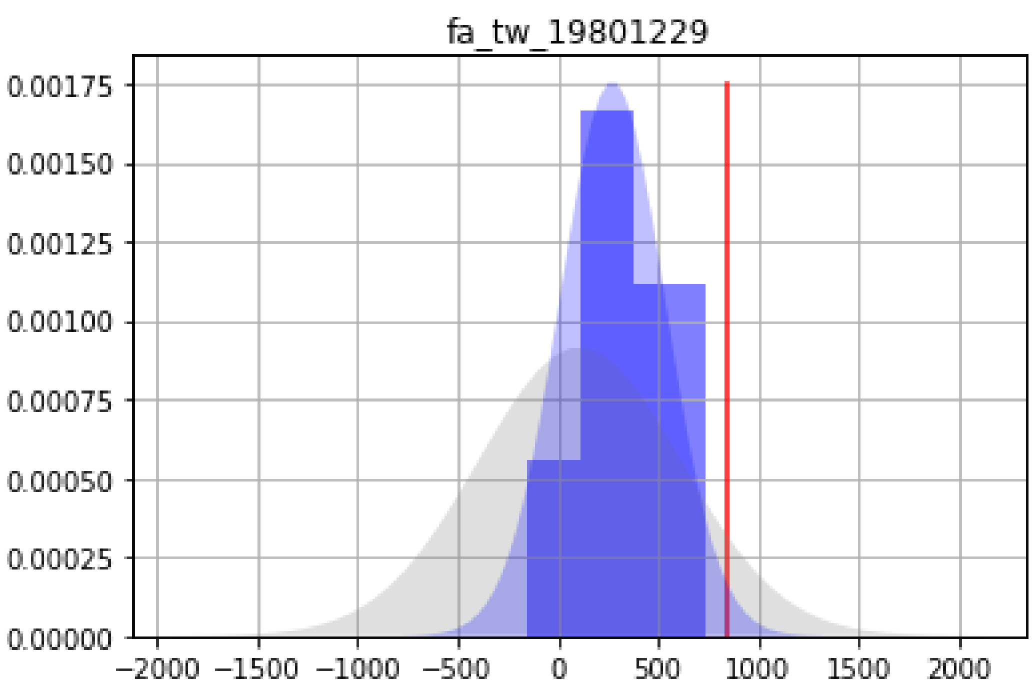
In [28]:
```
obs = pst.observation_data
fnames = pst.pestpp_options["forecasts"].split(",")
for forecast in fnames:
    ax = plt.subplot(111)
    oe_pt.loc[:,forecast].hist(ax=ax,color="b",alpha=0.5,normed=True)
    ax.plot([obs.loc[forecast,"obsval"],obs.loc[forecast,"obsval"]],ax.get_ylim(),"r"
  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

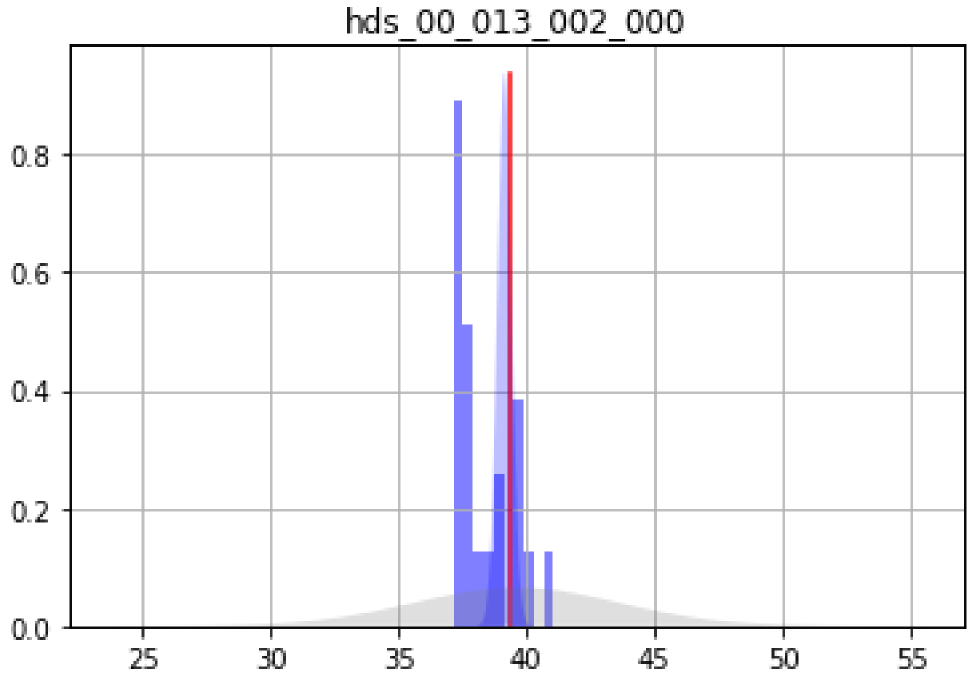
```
axt.set_ylim(0,axt.get_ylim()[1])
axt.set_yticks([])
ax.set_title(forecast)
plt.show()
```

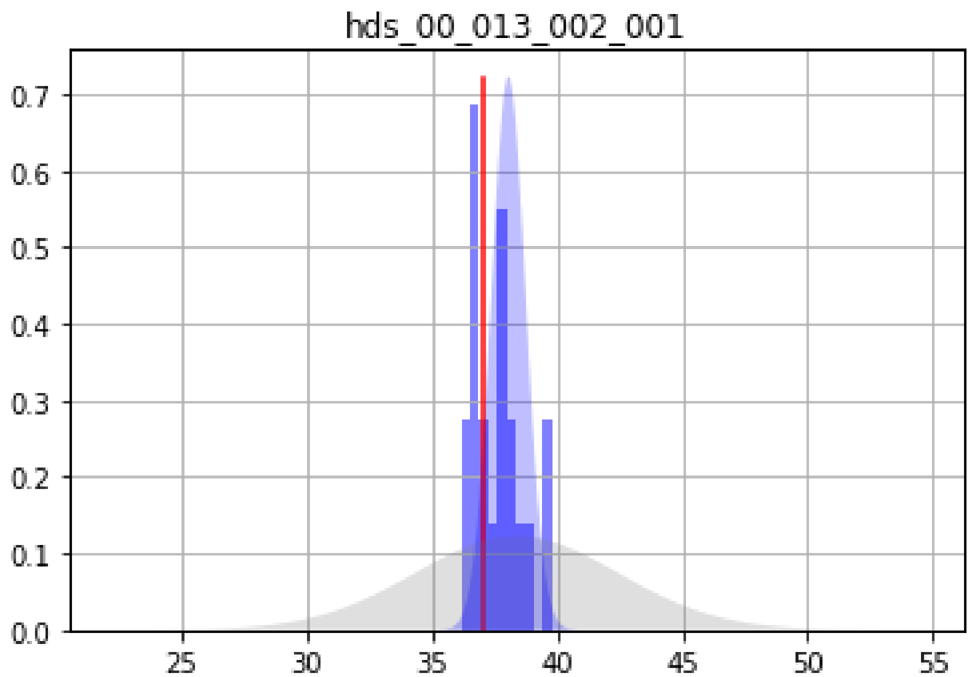


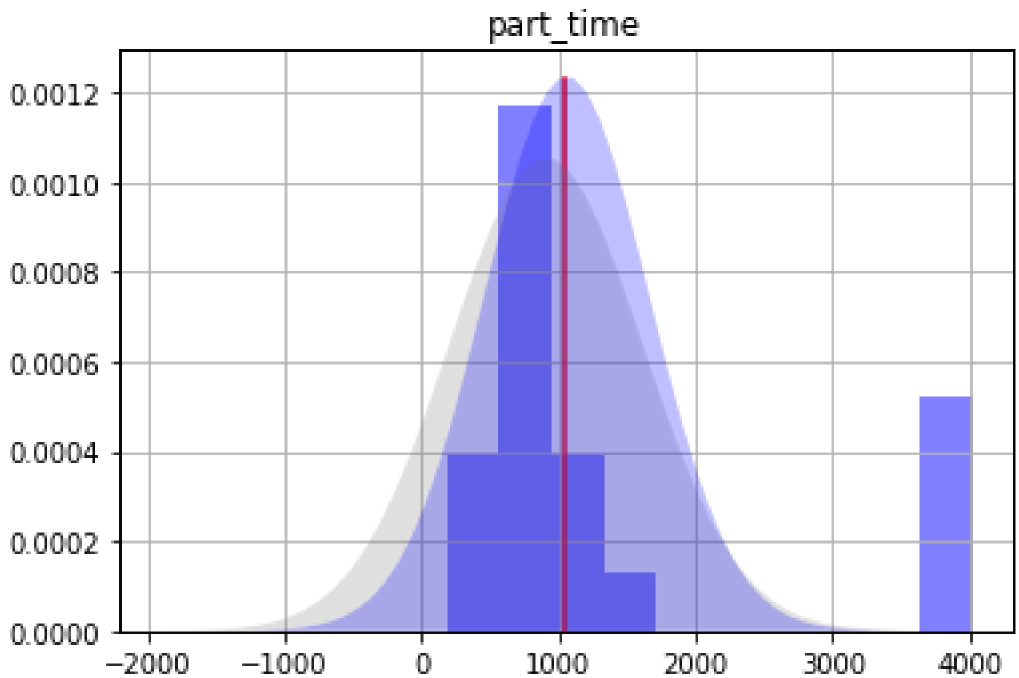


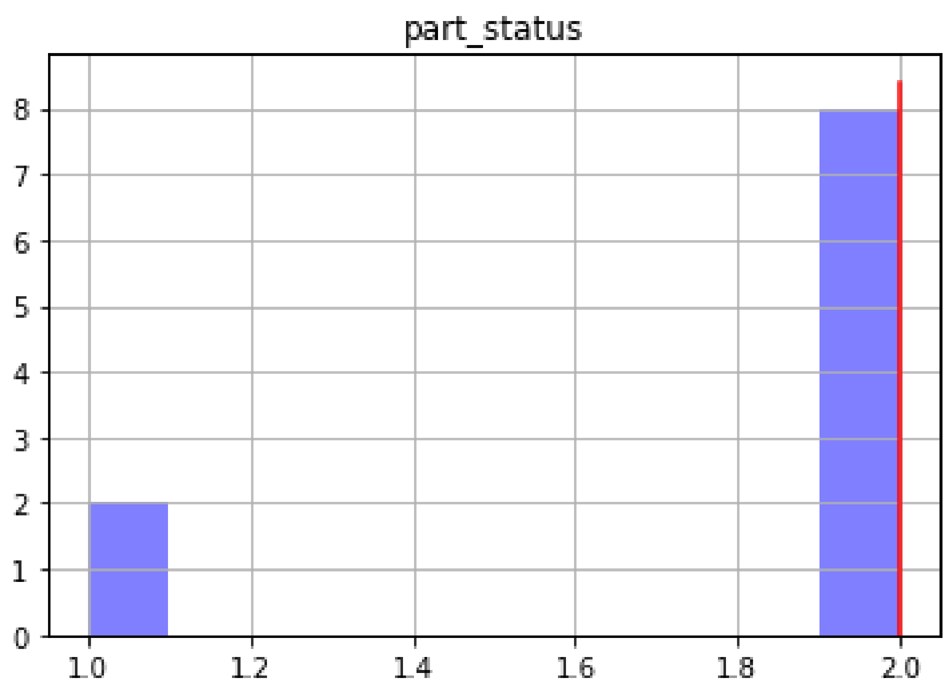

fa_tw_19791230
0.0035
0.0030
0.0025
0.0020
0.0015
0.0010
0.0005
0.0000
−2000
−1500
−1000
−500
0
500
1000


fa_tw_19801229
0.00175
0.00150
0.00125
0.00100
0.00075
0.00050
0.00025
0.00000
−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
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0.0
25
30
35
40
45
50
55


part_time
0.0012
0.0010
0.0008
0.0006
0.0004
0.0002
0.0000
−2000
−1000
0
1000
2000
3000
4000


part_status
8
7
6
5
4
3
2
1
0
1.0
1.2
1.4
1.6
1.8
2.0