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  \
        gr_vka4           gr_vka4       log    705                  0
        cn_vka7           cn_vka7       log      1                  0
        welflux           welflux       log      2      0 to 0.176091
        gr_rech2         gr_rech2       log    705                  0
        pp_vka0           pp_vka0       log     32                  0
        gr_sy5             gr_sy5       log    705                  0
        gr_ss3             gr_ss3       log    705                  0
        gr_vka5           gr_vka5       log    705                  0
        cn_vka8           cn_vka8       log      1                  0
        cn_hk6             cn_hk6       log      1                  0
        cn_rech4         cn_rech4       log      1                  0
        drncond_k00   drncond_k00       log     10                  0
        pp_hk1             pp_hk1       log     32                  0
```

gr_sy4	gr_sy4	log	705	0
flow	flow	log	1	0
cn_ss6	cn_ss6	log	1	0
strk	strk	log	40	0
cn_strt6	cn_strt6	log	1	0
pp_prsity2	pp_prsity2	log	32	0
pp_sy1	pp_sy1	log	32	0
gr_strt4	gr_strt4	log	705	0
gr_hk5	gr_hk5	log	705	0
gr_hk4	gr_hk4	log	705	0
cn_sy7	cn_sy7	log	1	0
cn_ss7	cn_ss7	log	1	0
cn_ss8	cn_ss8	log	1	0
pp_strt0	pp_strt0	log	32	0
gr_prsity4	gr_prsity4	log	705	0
gr_rech3	gr_rech3	log	705	0
gr_hk3	gr_hk3	log	705	0
...	...	...	...	...
cn_hk8	cn_hk8	log	1	0
cn_prsity6	cn_prsity6	log	1	0
pp_ss0	pp_ss0	log	32	0
cn_prsity7	cn_prsity7	log	1	0
cn_rech5	cn_rech5	log	1	-0.39794
welflux_k02	welflux_k02	log	6	0
gr_vka3	gr_vka3	log	705	0
pp_prsity1	pp_prsity1	log	32	0
gr_strt3	gr_strt3	log	705	0
pp_hk0	pp_hk0	log	32	0
gr_ss5	gr_ss5	log	705	0
pp_ss2	pp_ss2	log	32	0
cn_sy6	cn_sy6	log	1	0
gr_prsity5	gr_prsity5	log	705	0
pp_vka2	pp_vka2	log	32	0
gr_sy3	gr_sy3	log	705	0
cn_hk7	cn_hk7	log	1	0
pp_rech0	pp_rech0	log	32	0
cn_strt8	cn_strt8	log	1	0
gr_ss4	gr_ss4	log	705	0
pp_ss1	pp_ss1	log	32	0
pp_sy2	pp_sy2	log	32	0
cn_sy8	cn_sy8	log	1	0
pp_hk2	pp_hk2	log	32	0
cn_prsity8	cn_prsity8	log	1	0
pp_rech1	pp_rech1	log	32	0
gr_strt5	gr_strt5	log	705	0
pp_prsity0	pp_prsity0	log	32	0
pp_strt2	pp_strt2	log	32	0
pp_sy0	pp_sy0	log	32	0

	upper bound	lower bound	standard deviation
gr_vka4	1	-1	0.5
cn_vka7	1	-1	0.5
welflux	0.176091 to 0.30103	-0.30103 to 0	0.0752575 to 0.11928
gr_rech2	0.0413927	-0.0457575	0.0217875
pp_vka0	1	-1	0.5
gr_sy5	0.243038	-0.60206	0.211275
gr_ss3	1	-1	0.5
gr_vka5	1	-1	0.5
cn_vka8	1	-1	0.5
cn_hk6	1	-1	0.5
cn_rech4	0.0791812	-0.09691	0.0440228
drncond_k00	1	-1	0.5
pp_hk1	1	-1	0.5
gr_sy4	0.243038	-0.60206	0.211275
flow	0.09691	-0.124939	0.0554622
cn_ss6	1	-1	0.5
strk	2	-2	1
cn_strt6	0.0211893	-0.0222764	0.0108664
pp_prsity2	0	-1	0.25
pp_sy1	0.243038	-0.60206	0.211275
gr_strt4	0.0211893	-0.0222764	0.0108664
gr_hk5	1	-1	0.5
gr_hk4	1	-1	0.5
cn_sy7	0.243038	-0.60206	0.211275
cn_ss7	1	-1	0.5
cn_ss8	1	-1	0.5
pp_strt0	0.0211893	-0.0222764	0.0108664
gr_prsity4	0	-1	0.25
gr_rech3	0.0413927	-0.0457575	0.0217875
gr_hk3	1	-1	0.5
...	...	...	...
cn_hk8	1	-1	0.5
cn_prsity6	0	-1	0.25
pp_ss0	1	-1	0.5
cn_prsity7	0	-1	0.25
cn_rech5	-0.09691	-1	0.225772
welflux_k02	1	-1	0.5
gr_vka3	1	-1	0.5
pp_prsity1	0	-1	0.25
gr_strt3	0.0211893	-0.0222764	0.0108664
pp_hk0	1	-1	0.5
gr_ss5	1	-1	0.5
pp_ss2	1	-1	0.5
cn_sy6	0.243038	-0.60206	0.211275
gr_prsity5	0	-1	0.25
pp_vka2	1	-1	0.5

```
gr_sy3                0.243038       -0.60206       0.211275
cn_hk7                       1             -1            0.5
pp_rech0             0.0413927     -0.0457575      0.0217875
cn_strt8             0.0211893     -0.0222764      0.0108664
gr_ss4                       1             -1            0.5
pp_ss1                       1             -1            0.5
pp_sy2                0.243038       -0.60206       0.211275
cn_sy8                0.243038       -0.60206       0.211275
pp_hk2                       1             -1            0.5
cn_prsity8                   0             -1           0.25
pp_rech1             0.0413927     -0.0457575      0.0217875
gr_strt5             0.0211893     -0.0222764      0.0108664
pp_prsity0                   0             -1           0.25
pp_strt2             0.0211893     -0.0222764      0.0108664
pp_sy0                0.243038       -0.60206       0.211275

[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_sy8          1
cn_rech4        1
cn_hk6          1
cn_ss6          1
cn_sy7          1
flow            1
cn_vka8         1
cn_vka7         1
cn_strt7        1
cn_strt6        1
cn_hk8          1
cn_prsity8      1
cn_rech5        1
cn_ss7          1
cn_strt8        1
cn_hk7          1
cn_vka6         1
cn_sy6          1
cn_prsity6      1
cn_ss8          1
cn_prsity7      1
welflux         2
welflux_k02     6
drncond_k00    10
pp_ss0         32
pp_sy0         32
pp_sy2         32
pp_vka0        32
pp_hk1         32
pp_prsity1     32
pp_prsity2     32
pp_rech1       32
pp_ss1         32
pp_sy1         32
pp_strt0       32
pp_vka1        32
pp_strt1       32
pp_ss2         32
```

```
pp_rech0       32
pp_prsity0     32
pp_hk0         32
pp_hk2         32
pp_vka2        32
pp_strt2       32
strk           40
Name: pargp, dtype: int64
```

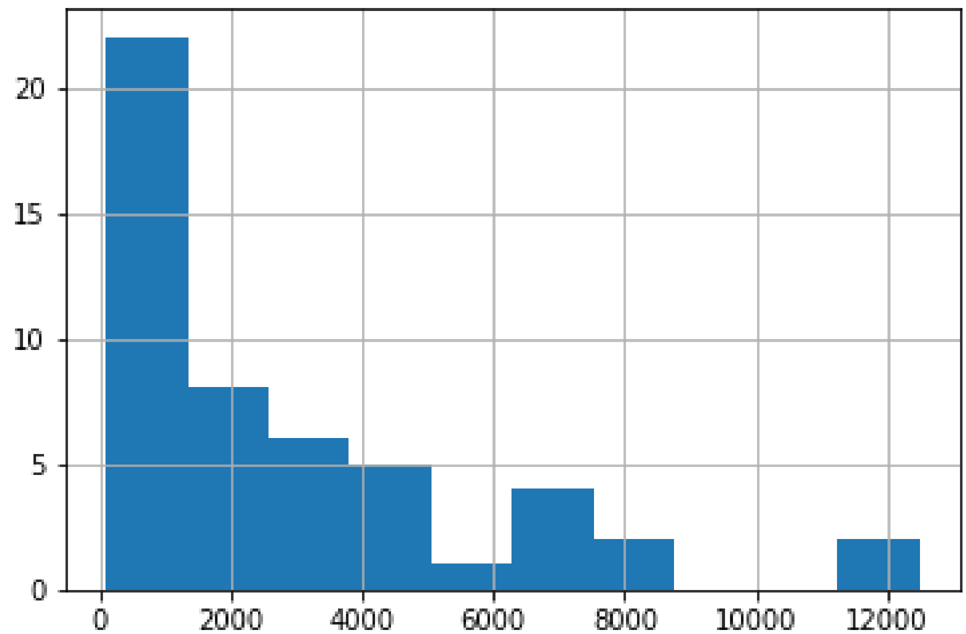
fix the future recharge pilot points, vka in layers 1 and 3 and the initial condition pilot points (we still have layer-scale pars for each of these types)

```
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
         21      105.630787
         33      250.056863
         15      341.328184
         45      341.959245
         5       361.923751
         23      361.985973
         36      379.002255
         19      433.680020
         35      435.836633
```

```
8       566.688279
48      575.856958
37      591.763851
7       682.465841
17      734.368859
39      803.951847
11      913.109707
10      936.800544
34      957.916272
1      1119.577753
49     1168.722748
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
```

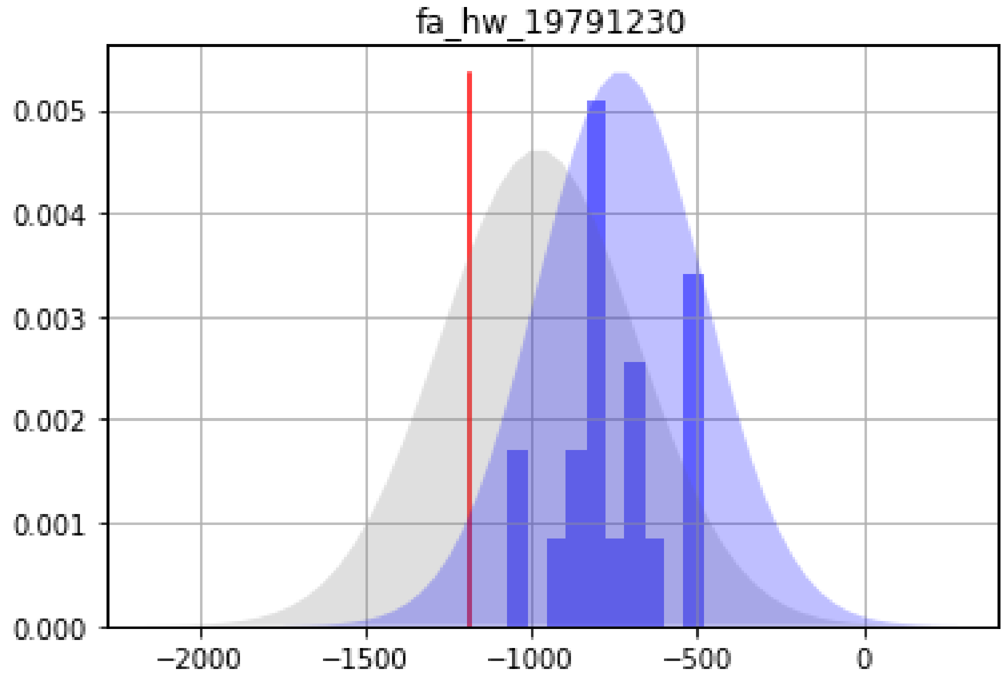
We can also load and plot the FOSM forecast results along side of the ensemble results:

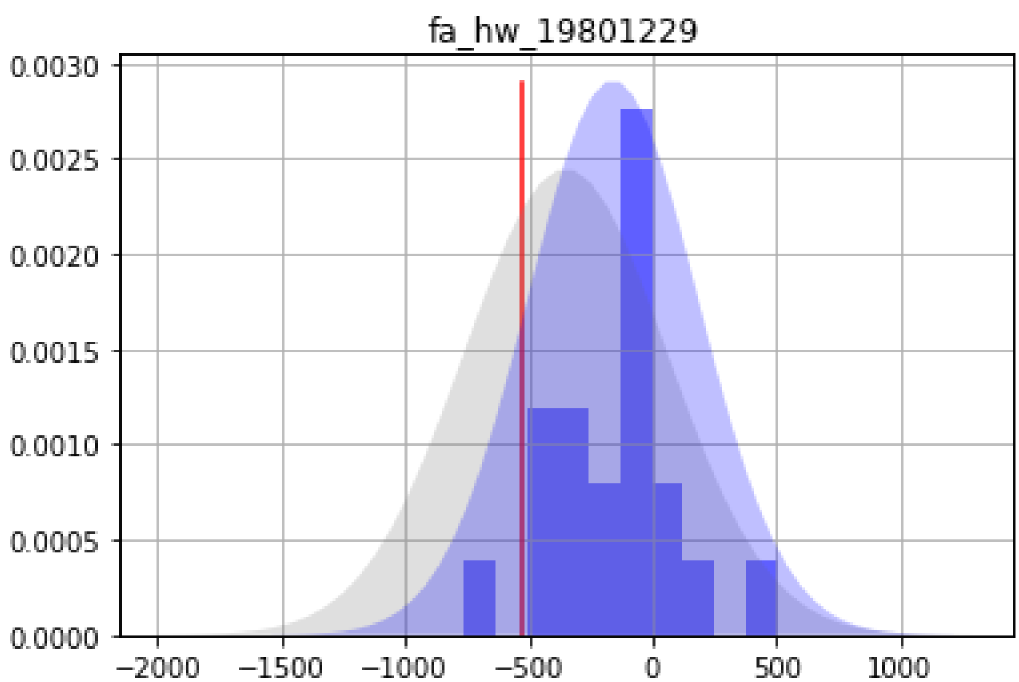
```
In [16]: f_df = pd.read_csv(os.path.join(m_d,"freyberg_pp.pred.usum.csv"),index_col=0)
         f_df.index = f_df.index.map(str.lower)
         f_df
```

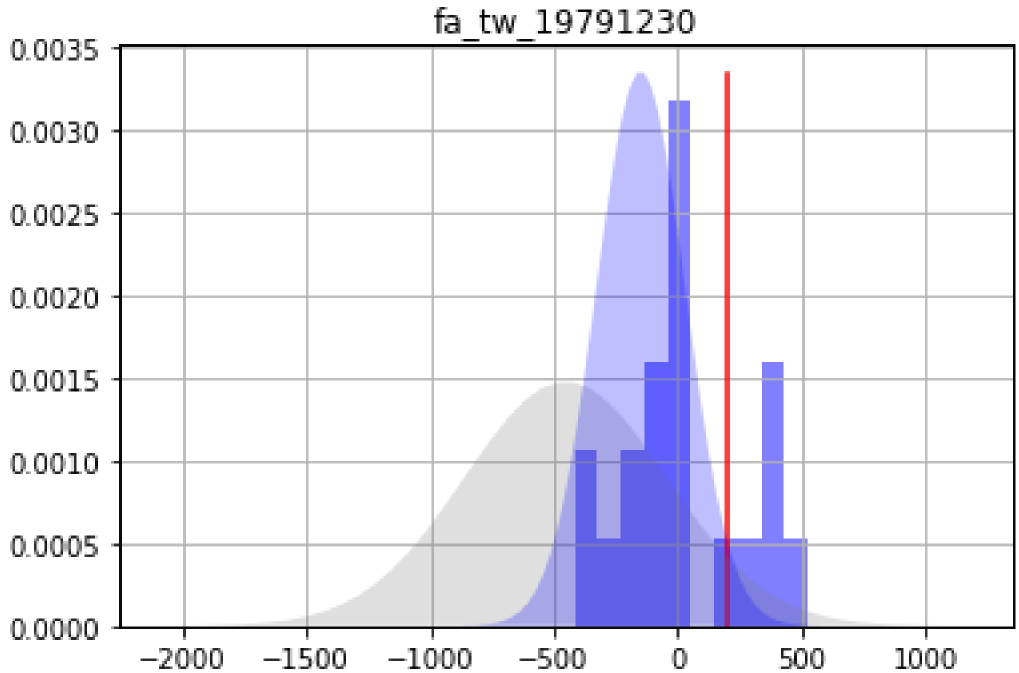
```
Out[16]:                          prior_mean  prior_stdev  prior_lower_bound  \
         name
```

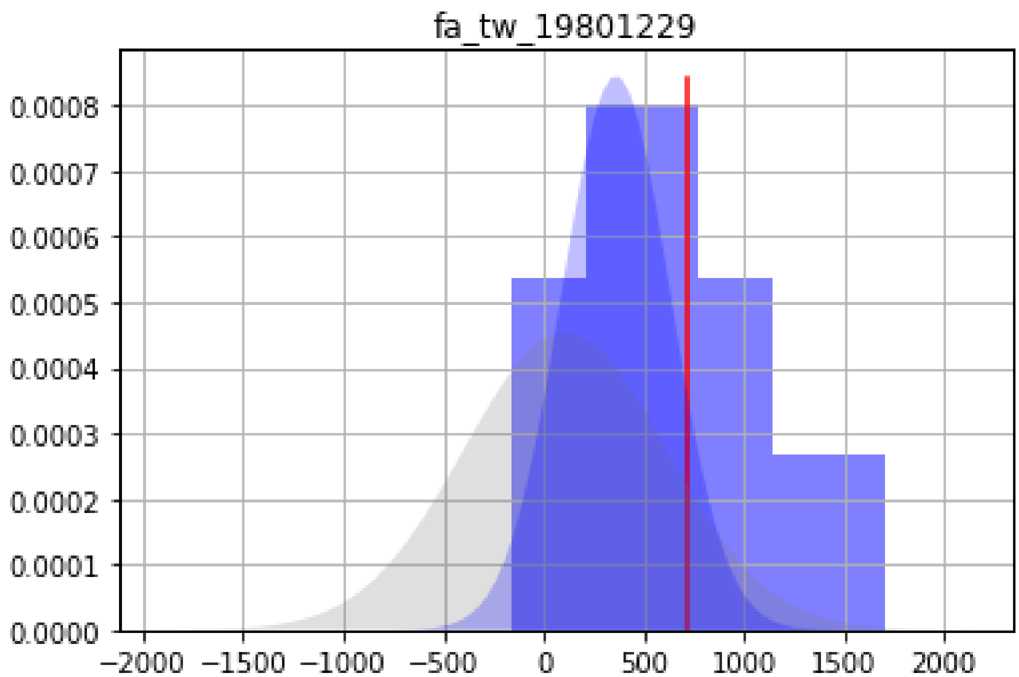
```
fa_hw_19791230        -977.2390    295.32800         -1567.8900
fa_hw_19801229        -351.2160    409.77000         -1170.7600
fa_tw_19791230        -453.0330    409.35100         -1271.7400
fa_tw_19801229         108.9600    506.73200          -904.5040
hds_00_013_002_000      39.6102      3.96314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

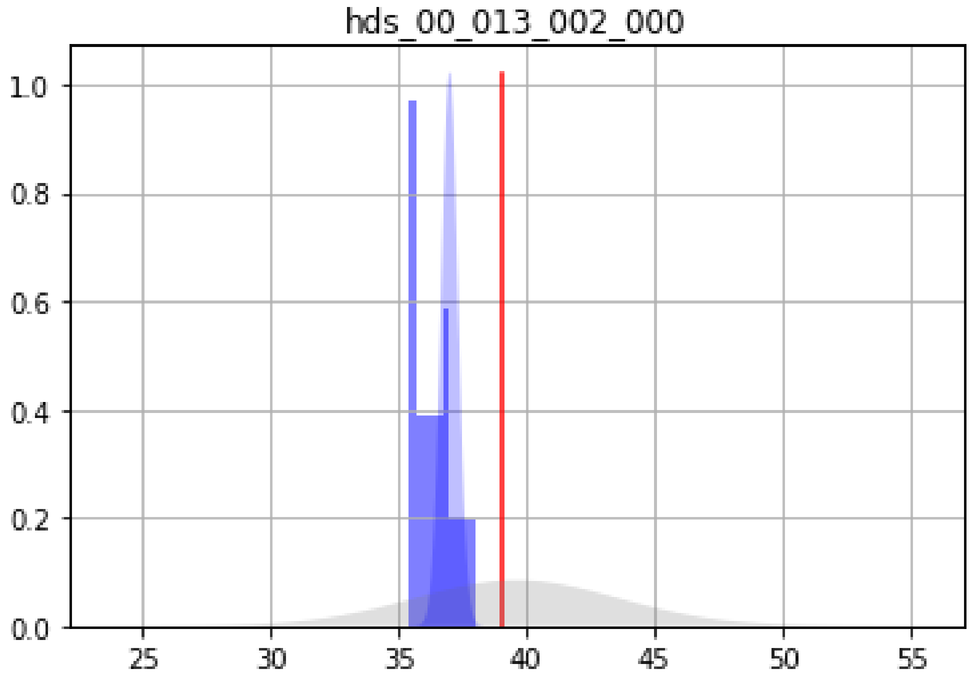
In [17]:
```python
obs = pst.observation_data
fnames = pst.pestpp_options["forecasts"].split(",")
for forecast in fnames:
    ax = plt.subplot(111)
    oe_pt.loc[:,forecast].hist(ax=ax,color="b",alpha=0.5,normed=True)
    ax.plot([obs.loc[forecast,"obsval"],obs.loc[forecast,"obsval"]],ax.get_ylim(),"r"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

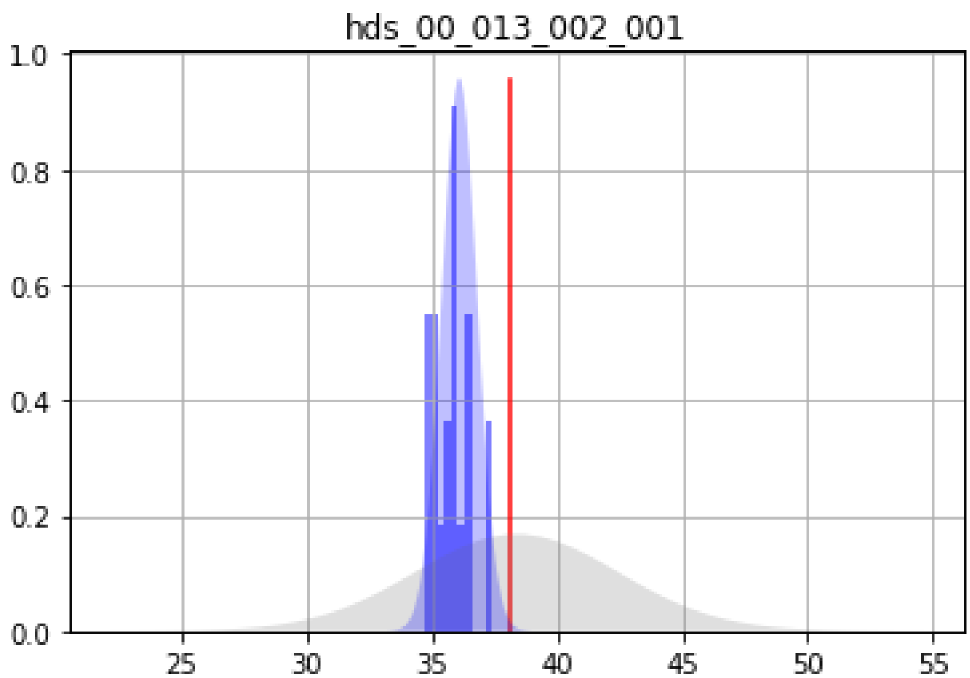

fa_hw_19791230
0.005
0.004
0.003
0.002
0.001
0.000
−2000
−1500
−1000
−500
0

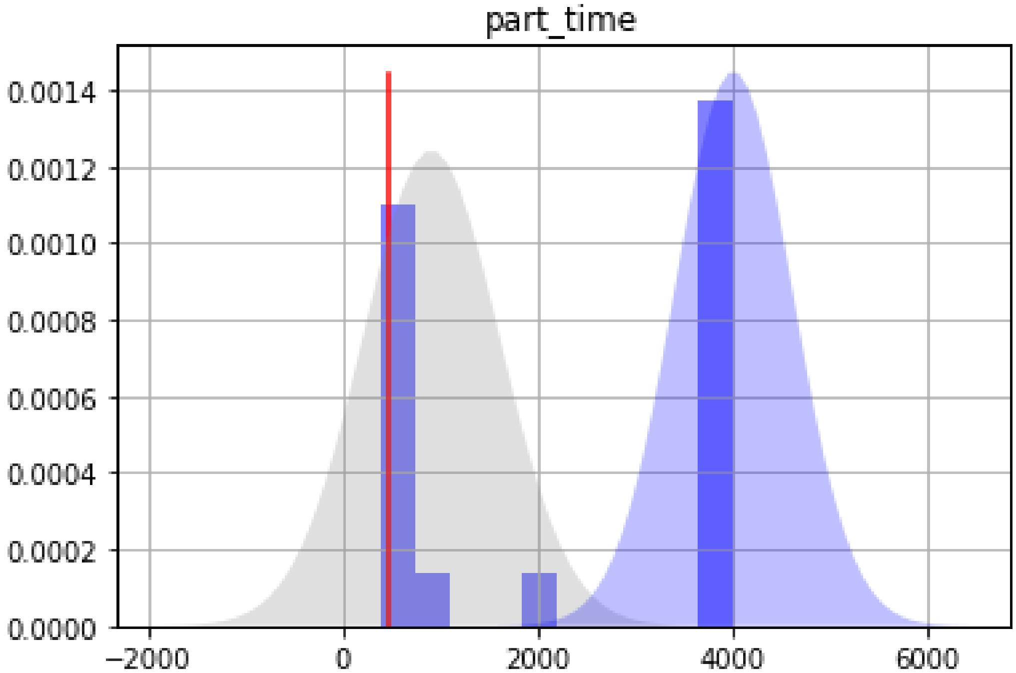

fa_hw_19801229
0.0030
0.0025
0.0020
0.0015
0.0010
0.0005
0.0000
−2000
−1500
−1000
−500
0
500
1000

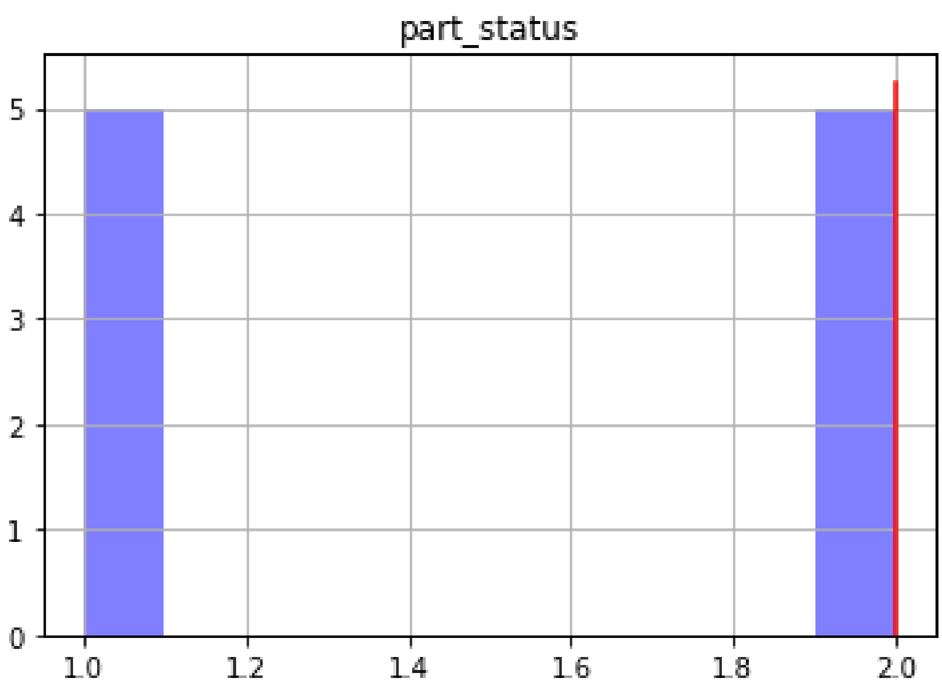

fa_tw_19791230
0.0035
0.0030
0.0025
0.0020
0.0015
0.0010
0.0005
0.0000
−2000
−1500
−1000
−500
0
500
1000


fa_tw_19801229
0.0008
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

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'
```

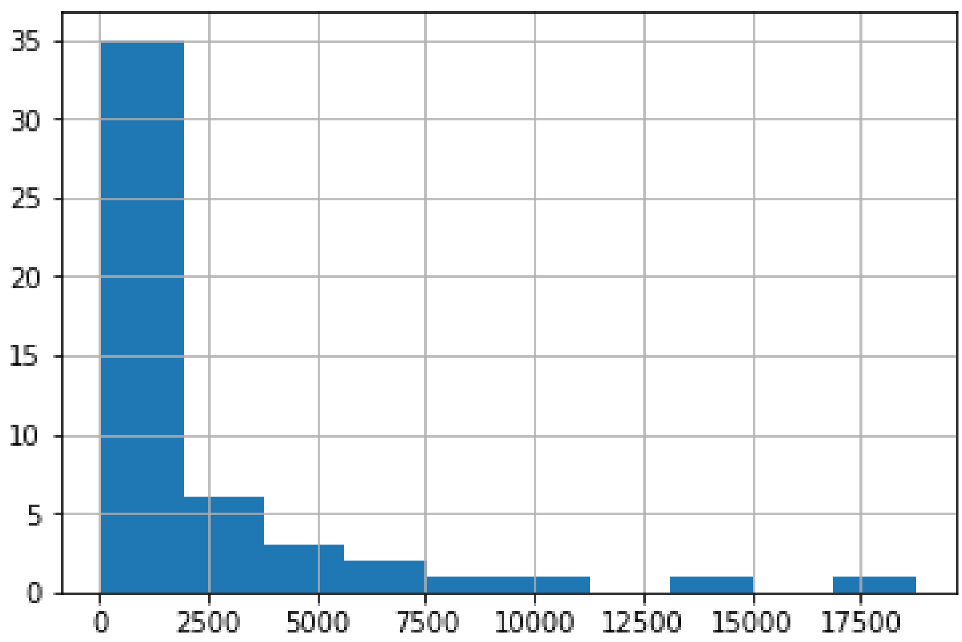
```
In [22]: pst.pestpp_options["base_jacobian"] = "restart_pp.jcb"
         pst.reg_data.phimlim = pst.nnz_obs
         pst.reg_data.phimaccept = pst.reg_data.phimlim * 1.1
         pst.write(os.path.join(t_d,"freyberg_pp.pst"))
```

```
In [23]: pyemu.os_utils.start_slaves(t_d,"pestpp-glm","freyberg_pp.pst",num_slaves=20,slave_roo
                                     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
         0      59.324204
         38     82.194416
         5      97.574472
         17    117.532065
         8     165.624313
         23    168.838806
         36    212.341022
         49    218.655514
         9     251.151530
         37    264.760800
         39    265.784626
         44    274.808989
         45    284.772193
         48    294.292926
         47    341.094426
         7     352.179906
         19    366.867432
         26    399.599443
         11    403.500953
         35    429.953038
         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:

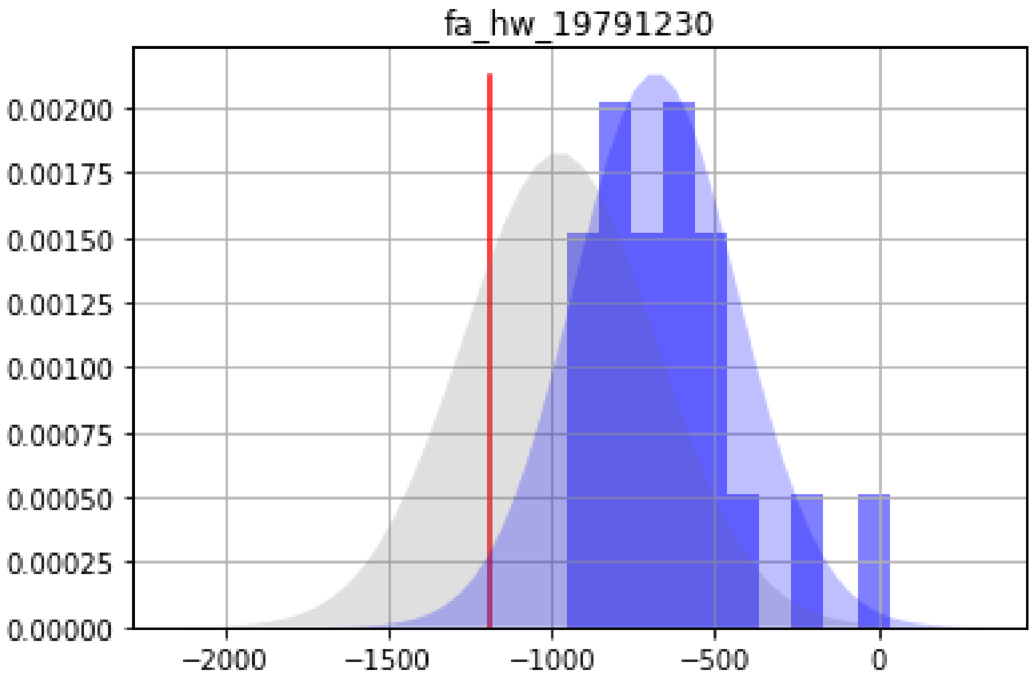
```
In [26]: oe_pt = oe.loc[oe.phi_vector.sort_values().index[:20],:]
```

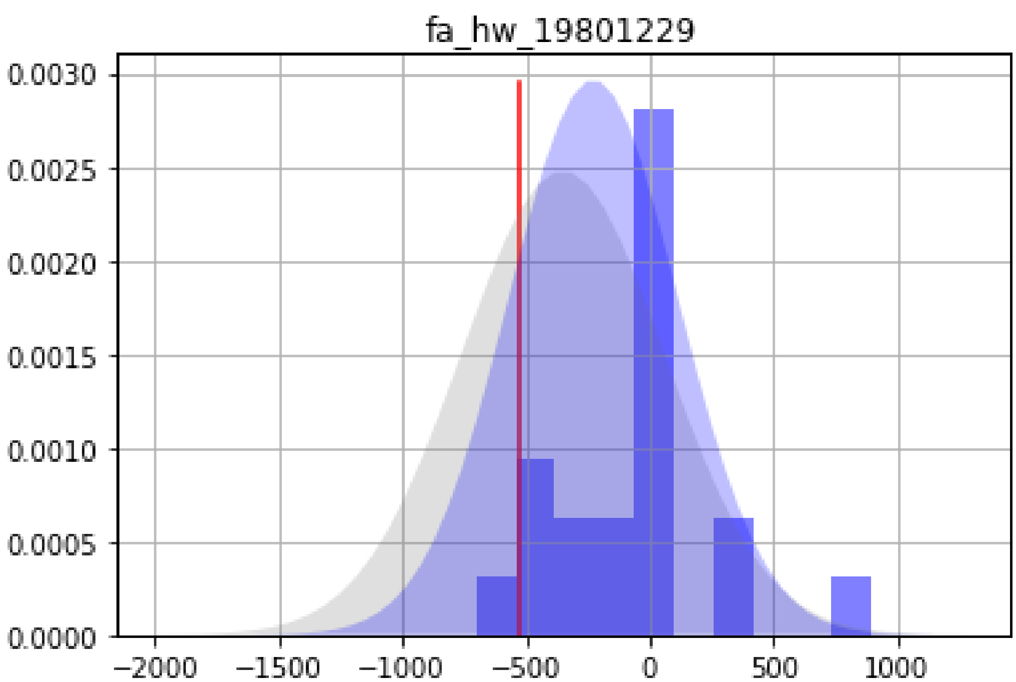
```
In [27]: f_df = pd.read_csv(os.path.join(m_d,"freyberg_pp.pred.usum.csv"),index_col=0)
         f_df.index = f_df.index.map(str.lower)
         f_df
```

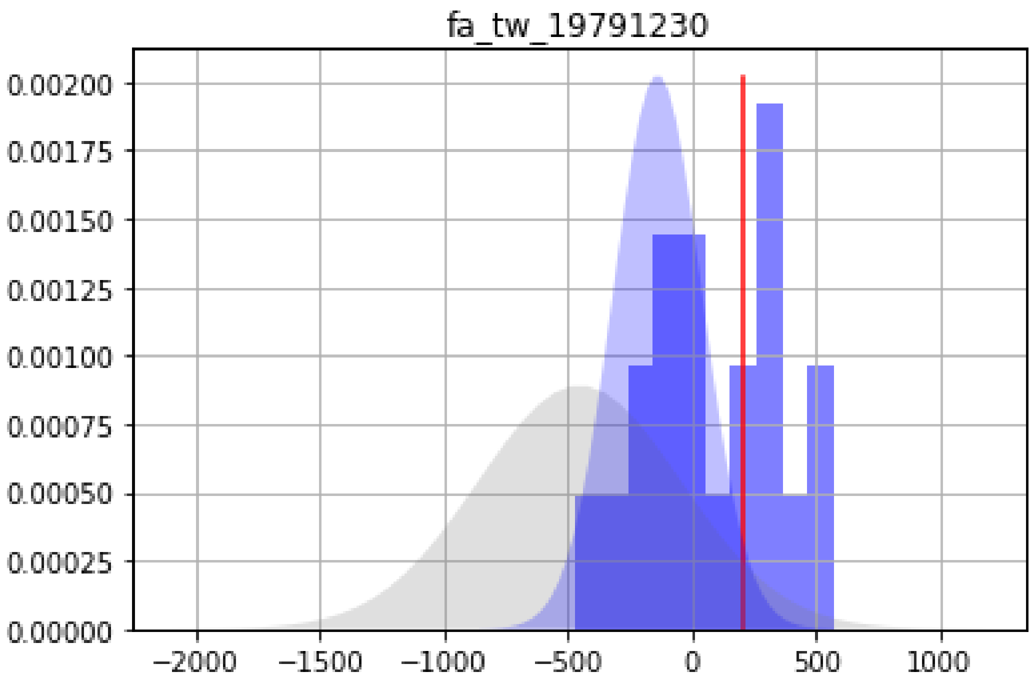
```
Out[27]:                     prior_mean  prior_stdev  prior_lower_bound  \
         name
         fa_hw_19791230       -977.2390    295.32800         -1567.8900
         fa_hw_19801229       -351.2160    409.77000         -1170.7600
         fa_tw_19791230       -453.0330    409.35100         -1271.7400
         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  -682.3380  252.978000
         fa_hw_19801229               468.3240  -227.9100  342.479000
         fa_tw_19791230               365.6690  -138.5270  179.850000
         fa_tw_19801229              1122.4200   264.8790  272.352000
         hds_00_013_002_000            47.5365    38.8495    0.409407
         hds_00_013_002_001            46.4994    37.7571    0.749881
         part_status                    2.0000     2.0000    0.000000
         part_time                   2317.2000  1059.5000  604.211000

                             post_lower_bound  post_upper_bound
         name
         fa_hw_19791230             -1188.2900         -176.3830
         fa_hw_19801229              -912.8690          457.0490
         fa_tw_19791230              -498.2270          221.1720
         fa_tw_19801229              -279.8240          809.5820
         hds_00_013_002_000            38.0307           39.6683
         hds_00_013_002_001            36.2573           39.2568
         part_status                    2.0000            2.0000
         part_time                   -148.9210         2267.9200
```

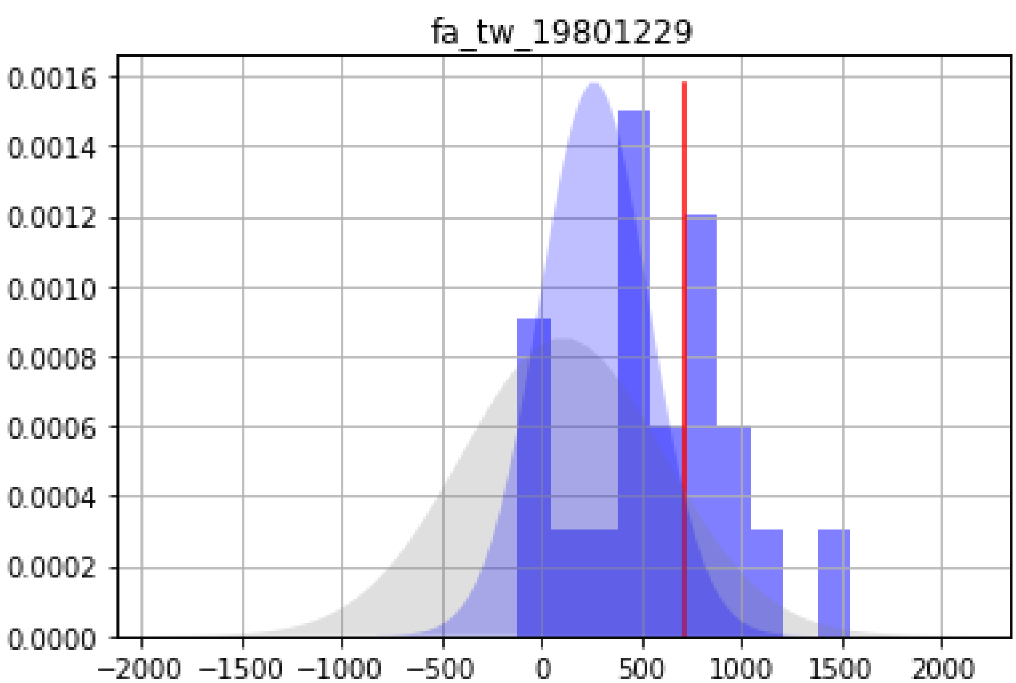
```
In [28]: obs = pst.observation_data
         fnames = pst.pestpp_options["forecasts"].split(",")
         for forecast in fnames:
             ax = plt.subplot(111)
             oe_pt.loc[:,forecast].hist(ax=ax,color="b",alpha=0.5,normed=True)
             ax.plot([obs.loc[forecast,"obsval"],obs.loc[forecast,"obsval"]],ax.get_ylim(),"r"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

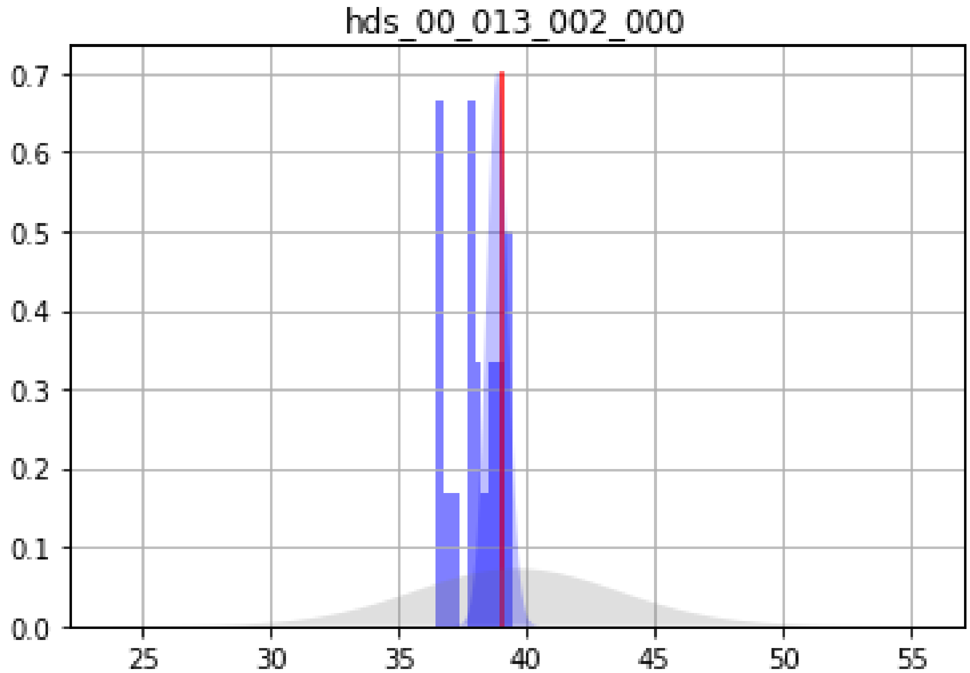
```
axt.set_ylim(0,axt.get_ylim()[1])
axt.set_yticks([])
ax.set_title(forecast)
plt.show()
```

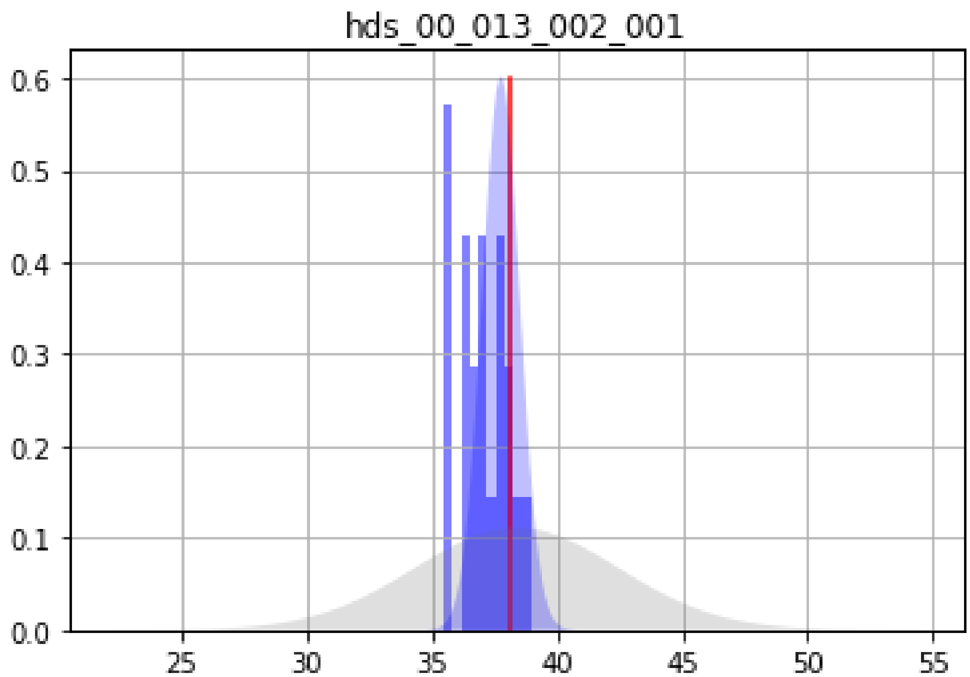


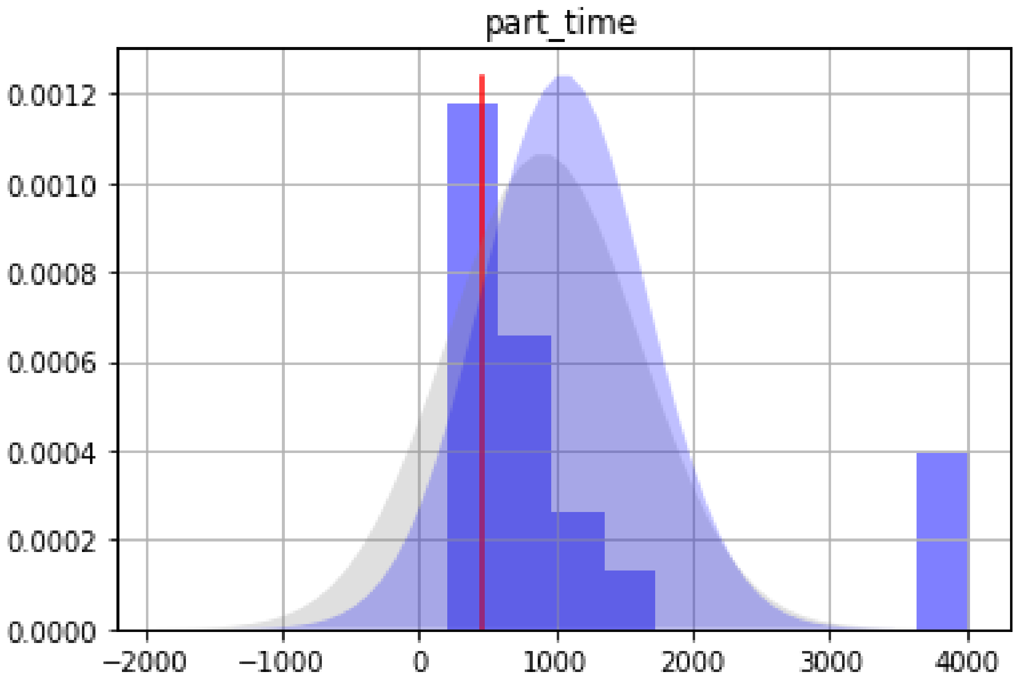


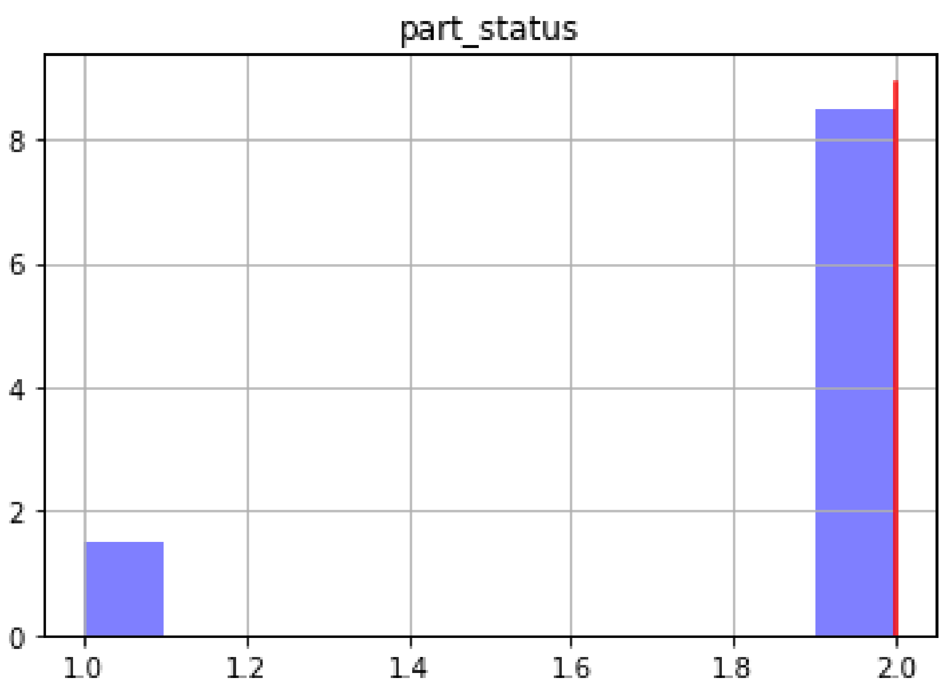

fa_tw_19791230
0.00200
0.00175
0.00150
0.00125
0.00100
0.00075
0.00050
0.00025
0.00000
−2000
−1500
−1000
−500
0
500
1000


fa_tw_19801229
0.0016
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
0.7
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
0.6
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
6
4
2
0
1.0
1.2
1.4
1.6
1.8
2.0