pestpp-glm

May 7, 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
```

```
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_prsity4    gr_prsity4       log    705                  0
        cn_sy8             cn_sy8       log      1                  0
        cn_ss8             cn_ss8       log      1                  0
        gr_strt4         gr_strt4       log    705                  0
        gr_rech3         gr_rech3       log    705                  0
        pp_hk2             pp_hk2       log     32                  0
        gr_ss3             gr_ss3       log    705                  0
        gr_hk3             gr_hk3       log    705                  0
        pp_ss2             pp_ss2       log     32                  0
        gr_sy5             gr_sy5       log    705                  0
        gr_ss5             gr_ss5       log    705                  0
```

cn_strt6	cn_strt6	log	1	0
gr_prsity5	gr_prsity5	log	705	0
pp_sy2	pp_sy2	log	32	0
pp_hk0	pp_hk0	log	32	0
strk	strk	log	40	0
cn_sy6	cn_sy6	log	1	0
gr_strt5	gr_strt5	log	705	0
gr_prsity3	gr_prsity3	log	705	0
drncond_k00	drncond_k00	log	10	0
cn_prsity7	cn_prsity7	log	1	0
cn_vka6	cn_vka6	log	1	0
gr_rech2	gr_rech2	log	705	0
gr_sy3	gr_sy3	log	705	0
pp_strt0	pp_strt0	log	32	0
pp_strt2	pp_strt2	log	32	0
pp_hk1	pp_hk1	log	32	0
gr_strt3	gr_strt3	log	705	0
gr_sy4	gr_sy4	log	705	0
gr_vka3	gr_vka3	log	705	0
...	...	...	...	...
pp_strt1	pp_strt1	log	32	0
cn_rech5	cn_rech5	log	1	-0.39794
cn_strt8	cn_strt8	log	1	0
flow	flow	log	1	0
gr_ss4	gr_ss4	log	705	0
cn_rech4	cn_rech4	log	1	0
cn_vka7	cn_vka7	log	1	0
gr_vka5	gr_vka5	log	705	0
gr_hk4	gr_hk4	log	705	0
cn_prsity8	cn_prsity8	log	1	0
pp_prsity2	pp_prsity2	log	32	0
pp_prsity0	pp_prsity0	log	32	0
pp_vka2	pp_vka2	log	32	0
cn_hk6	cn_hk6	log	1	0
welflux_k02	welflux_k02	log	6	0
cn_hk7	cn_hk7	log	1	0
cn_vka8	cn_vka8	log	1	0
gr_hk5	gr_hk5	log	705	0
cn_ss7	cn_ss7	log	1	0
pp_sy0	pp_sy0	log	32	0
cn_hk8	cn_hk8	log	1	0
pp_vka1	pp_vka1	log	32	0
pp_prsity1	pp_prsity1	log	32	0
cn_strt7	cn_strt7	log	1	0
pp_rech1	pp_rech1	log	32	0
cn_sy7	cn_sy7	log	1	0
cn_ss6	cn_ss6	log	1	0
pp_ss0	pp_ss0	log	32	0

pp_vka0	pp_vka0	log	32	0
welflux	welflux	log	2	0 to 0.176091

	upper bound	lower bound	standard deviation
gr_prsity4	0	-1	0.25
cn_sy8	0.243038	-0.60206	0.211275
cn_ss8	1	-1	0.5
gr_strt4	0.0211893	-0.0222764	0.0108664
gr_rech3	0.0413927	-0.0457575	0.0217875
pp_hk2	1	-1	0.5
gr_ss3	1	-1	0.5
gr_hk3	1	-1	0.5
pp_ss2	1	-1	0.5
gr_sy5	0.243038	-0.60206	0.211275
gr_ss5	1	-1	0.5
cn_strt6	0.0211893	-0.0222764	0.0108664
gr_prsity5	0	-1	0.25
pp_sy2	0.243038	-0.60206	0.211275
pp_hk0	1	-1	0.5
strk	2	-2	1
cn_sy6	0.243038	-0.60206	0.211275
gr_strt5	0.0211893	-0.0222764	0.0108664
gr_prsity3	0	-1	0.25
drncond_k00	1	-1	0.5
cn_prsity7	0	-1	0.25
cn_vka6	1	-1	0.5
gr_rech2	0.0413927	-0.0457575	0.0217875
gr_sy3	0.243038	-0.60206	0.211275
pp_strt0	0.0211893	-0.0222764	0.0108664
pp_strt2	0.0211893	-0.0222764	0.0108664
pp_hk1	1	-1	0.5
gr_strt3	0.0211893	-0.0222764	0.0108664
gr_sy4	0.243038	-0.60206	0.211275
gr_vka3	1	-1	0.5
...	...	...	...
pp_strt1	0.0211893	-0.0222764	0.0108664
cn_rech5	-0.09691	-1	0.225772
cn_strt8	0.0211893	-0.0222764	0.0108664
flow	0.09691	-0.124939	0.0554622
gr_ss4	1	-1	0.5
cn_rech4	0.0791812	-0.09691	0.0440228
cn_vka7	1	-1	0.5
gr_vka5	1	-1	0.5
gr_hk4	1	-1	0.5
cn_prsity8	0	-1	0.25
pp_prsity2	0	-1	0.25
pp_prsity0	0	-1	0.25
pp_vka2	1	-1	0.5

```
cn_hk6                        1              -1                0.5
welflux_k02                   1              -1                0.5
cn_hk7                        1              -1                0.5
cn_vka8                       1              -1                0.5
gr_hk5                        1              -1                0.5
cn_ss7                        1              -1                0.5
pp_sy0                 0.243038        -0.60206           0.211275
cn_hk8                        1              -1                0.5
pp_vka1                       1              -1                0.5
pp_prsity1                    0              -1               0.25
cn_strt7              0.0211893      -0.0222764          0.0108664
pp_rech1              0.0413927      -0.0457575          0.0217875
cn_sy7                 0.243038        -0.60206           0.211275
cn_ss6                        1              -1                0.5
pp_ss0                        1              -1                0.5
pp_vka0                       1              -1                0.5
welflux     0.176091 to 0.30103  -0.30103 to    0  0.0752575 to 0.11928

[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_ss8          1
cn_strt6        1
cn_strt8        1
cn_rech4        1
cn_prsity7      1
cn_prsity6      1
cn_sy6          1
cn_vka6         1
cn_vka7         1
cn_prsity8      1
flow            1
cn_hk6          1
cn_hk7          1
cn_vka8         1
cn_rech5        1
cn_hk8          1
cn_strt7        1
cn_sy7          1
cn_ss7          1
cn_ss6          1
welflux         2
welflux_k02     6
drncond_k00    10
pp_hk2         32
pp_strt2       32
pp_hk0         32
pp_hk1         32
pp_vka2        32
pp_rech0       32
pp_strt1       32
pp_vka0        32
pp_prsity0     32
pp_ss0         32
pp_rech1       32
pp_vka1        32
pp_sy2         32
pp_strt0       32
```

```
pp_sy1         32
pp_sy0         32
pp_ss2         32
pp_prsity1     32
pp_ss1         32
pp_prsity2     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"))
```

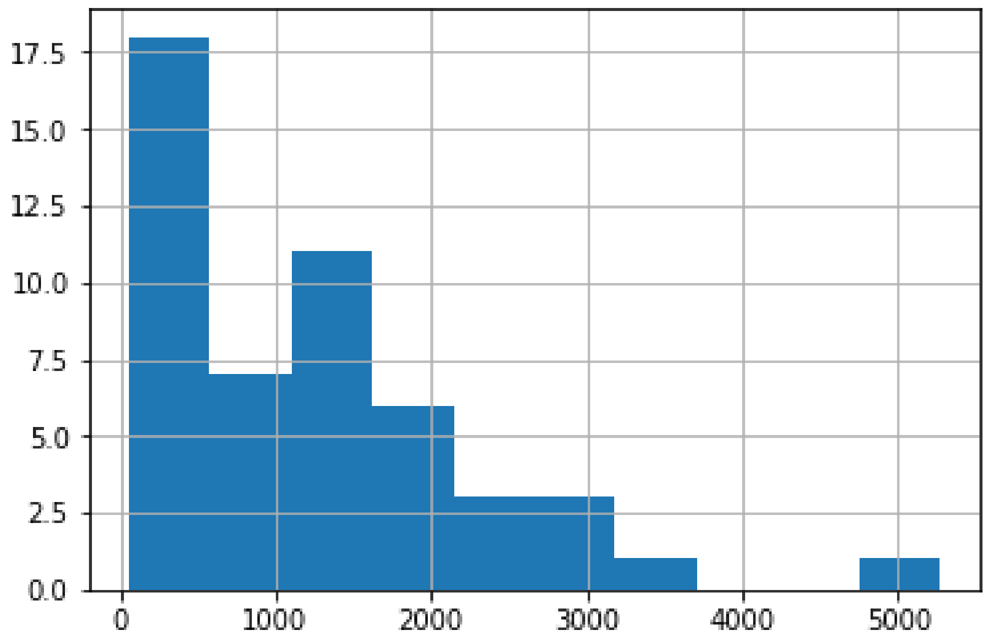
```
In [12]: pyemu.os_utils.start_slaves(t_d,"pestpp-glm","freyberg_pp.pst",num_slaves=20,slave_ro
                                     master_dir=m_d)
```

```
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       55.468202
         24      84.260295
         4      124.191279
         1      168.977488
         25     174.596536
         21     199.858942
         39     205.571352
         20     373.756778
         42     385.789083
```

```
12    428.295418
6     429.258788
16    430.476563
45    462.553423
19    495.599815
41    510.791903
22    512.655947
48    552.963192
33    573.280556
3     615.596134
37    772.791092
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
```

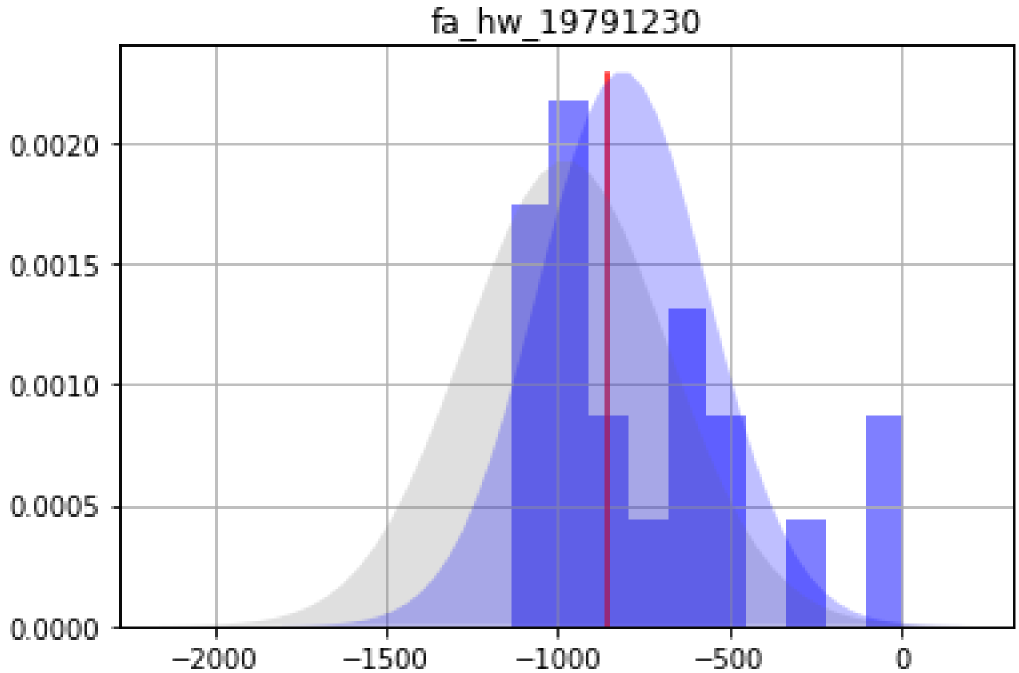
We can also load and plot the FOSM forecast results along side of the ensemble results:

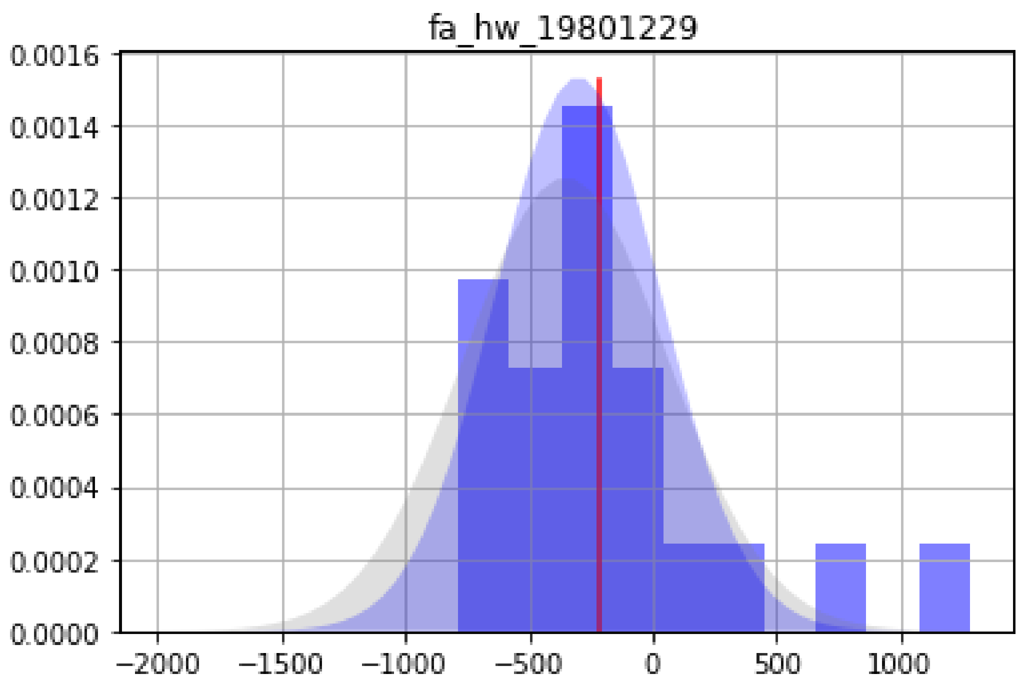
In [16]:
```
f_df = pd.read_csv(os.path.join(m_d,"freyberg_pp.pred.usum.csv"),index_col=0)
f_df.index = f_df.index.map(str.lower)
f_df
```

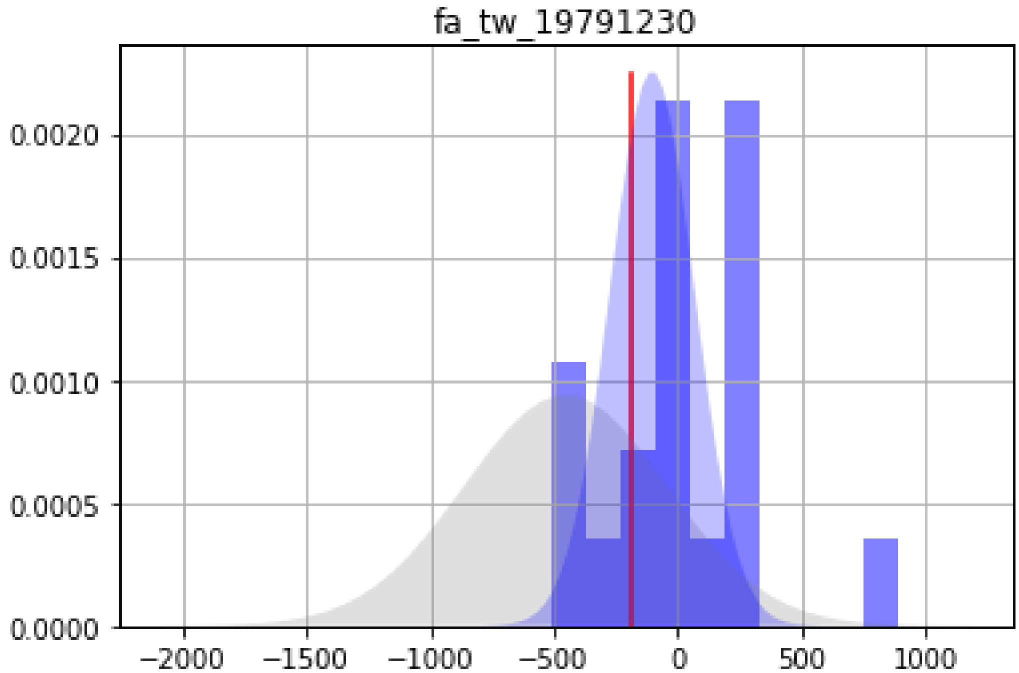
Out[16]:
```
                         prior_mean  prior_stdev  prior_lower_bound  \
name
```

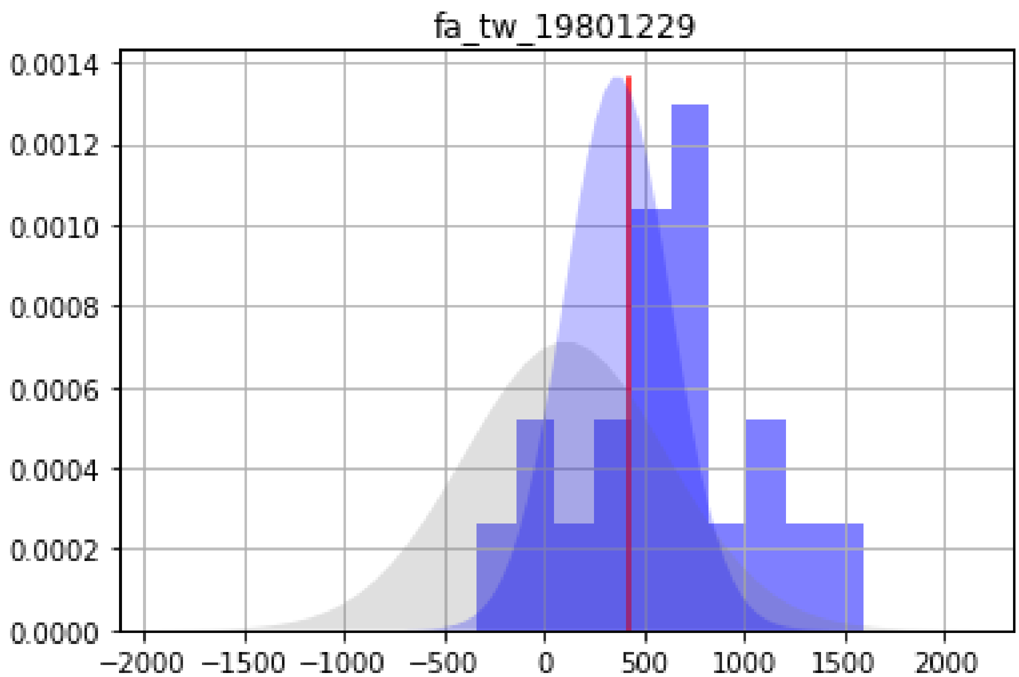
```
fa_hw_19791230       -977.2390    295.32800         -1567.8900
fa_hw_19801229       -351.2160    409.77000         -1170.7600
fa_tw_19791230       -453.0330    409.35100         -1271.7400
fa_tw_19801229        108.9600    506.73200          -904.5040
hds_00_013_002_000     39.6102      3.96314           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  -811.3660  247.865000
fa_hw_19801229               468.3240  -300.1030  335.551000
fa_tw_19791230               365.6690  -103.5390  170.577000
fa_tw_19801229              1122.4200   366.6750  263.681000
hds_00_013_002_000            47.5365    39.4199    0.273990
hds_00_013_002_001            46.4994    38.1797    0.687836
part_status                    2.0000     2.0000    0.000000
part_time                   2317.2000   730.7160  601.308000

                    post_lower_bound  post_upper_bound
name
fa_hw_19791230             -1307.1000         -315.6370
fa_hw_19801229              -971.2060          371.0000
fa_tw_19791230              -444.6930          237.6160
fa_tw_19801229              -160.6870          894.0380
hds_00_013_002_000            38.8719           39.9679
hds_00_013_002_001            36.8040           39.5553
part_status                    2.0000            2.0000
part_time                   -471.9010         1933.3300
```

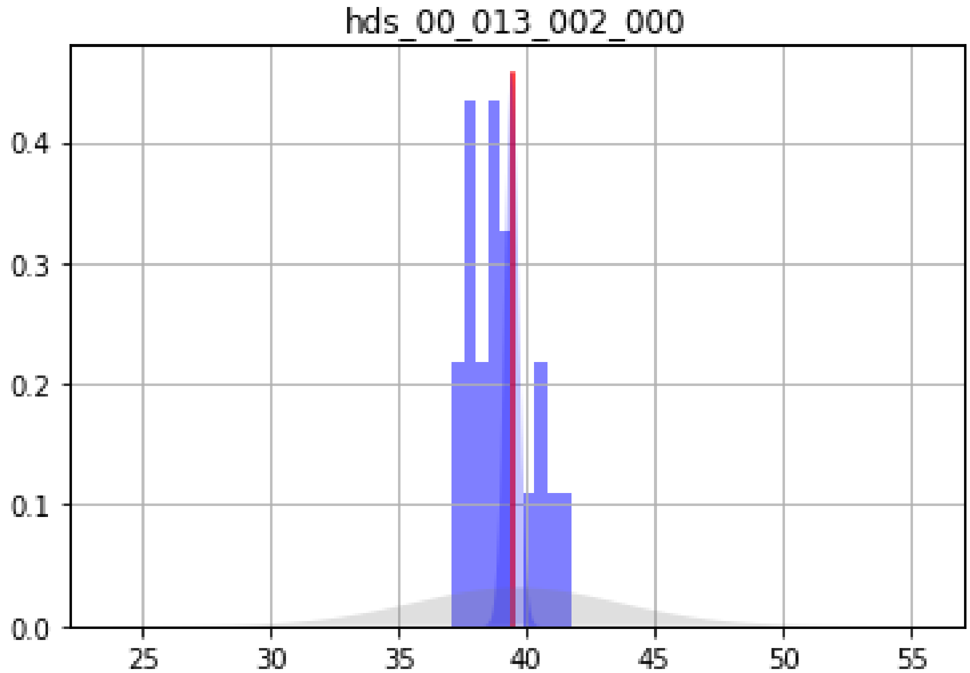
In [17]:
```
obs = pst.observation_data
fnames = pst.pestpp_options["forecasts"].split(",")
for forecast in fnames:
    ax = plt.subplot(111)
    oe_pt.loc[:,forecast].hist(ax=ax,color="b",alpha=0.5,normed=True)
    ax.plot([obs.loc[forecast,"obsval"],obs.loc[forecast,"obsval"]],ax.get_ylim(),"r"
  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

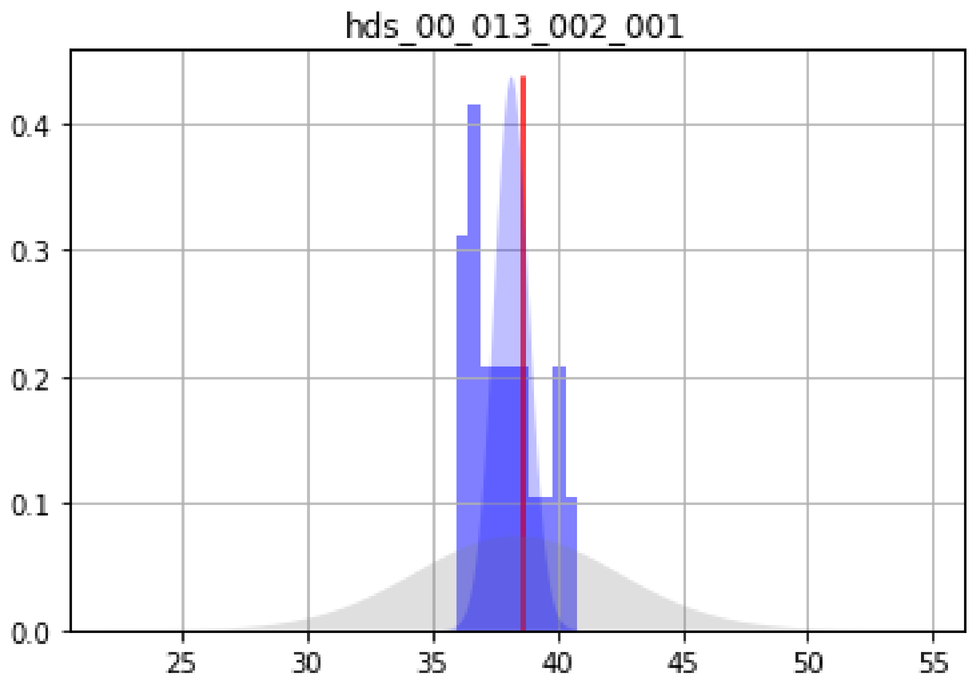

fa_hw_19791230
0.0020
0.0015
0.0010
0.0005
0.0000
−2000
−1500
−1000
−500
0

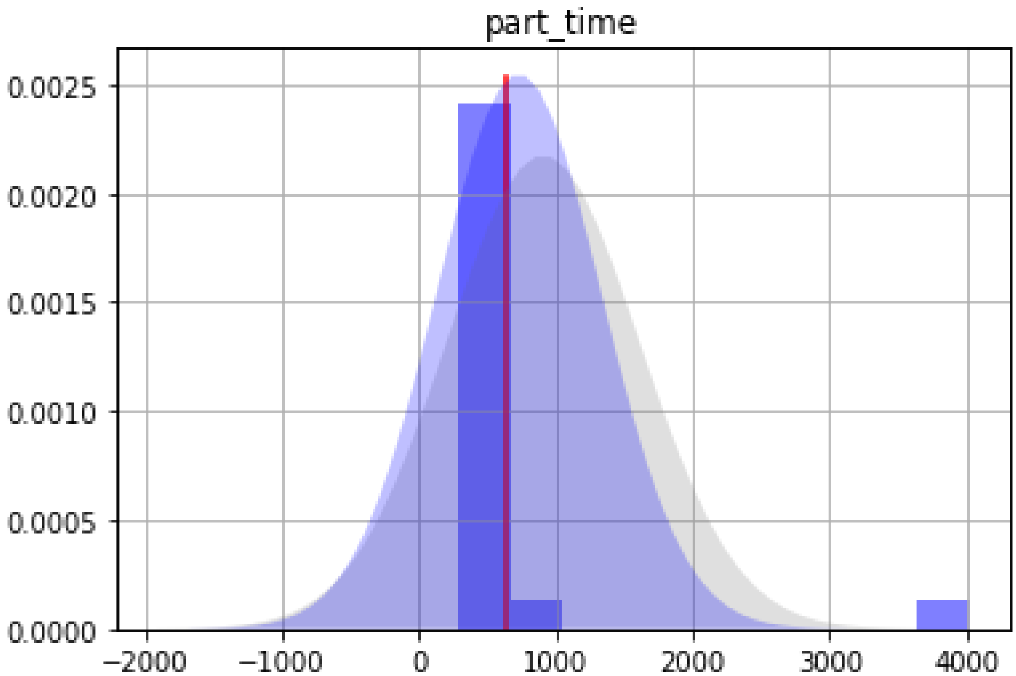

fa_hw_19801229
0.0016
0.0014
0.0012
0.0010
0.0008
0.0006
0.0004
0.0002
0.0000
−2000
−1500
−1000
−500
0
500
1000

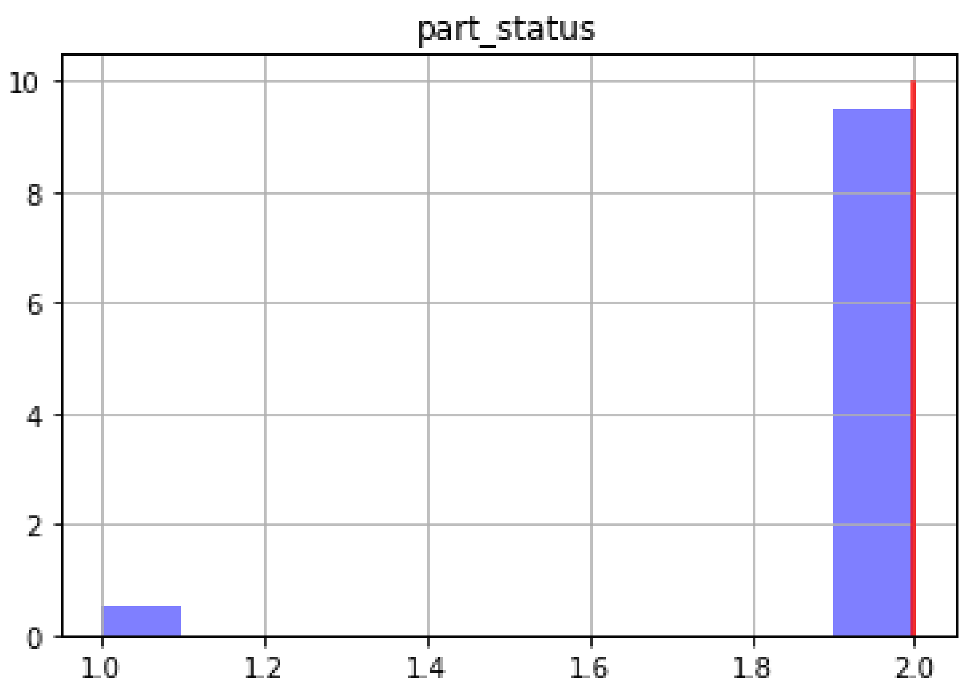

fa_tw_19791230
0.0020
0.0015
0.0010
0.0005
0.0000
−2000
−1500
−1000
−500
0
500
1000


fa_tw_19801229
0.0014
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
0.4
0.3
0.2
0.1
0.0
25
30
35
40
45
50
55


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


part_time
0.0025
0.0020
0.0015
0.0010
0.0005
0.0000
−2000
−1000
0
1000
2000
3000
4000


part_status
10
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'
```

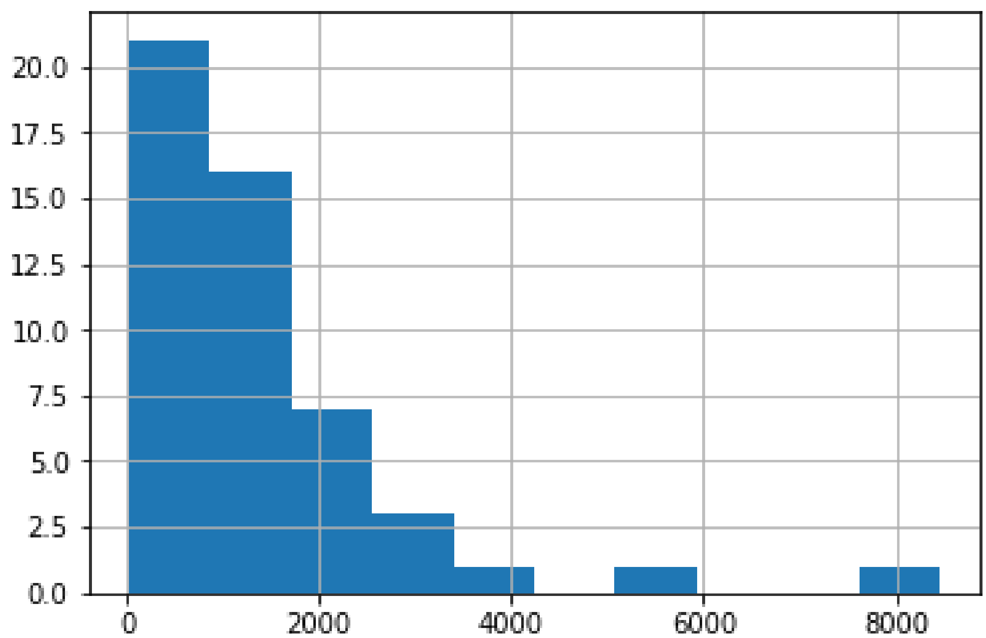
```
In [22]: pst.pestpp_options["base_jacobian"] = "restart_pp.jcb"
         pst.reg_data.phimlim = pst.nnz_obs
         pst.reg_data.phimaccept = pst.reg_data.phimlim * 1.1
         pst.write(os.path.join(t_d,"freyberg_pp.pst"))
```

```
In [23]: pyemu.os_utils.start_slaves(t_d,"pestpp-glm","freyberg_pp.pst",num_slaves=20,slave_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
         7      21.906757
         24     94.064807
         25    130.642360
         44    144.623771
         1     171.822277
         39    173.064244
         19    189.988899
         12    332.255646
         21    346.544001
         42    377.272242
         4     408.480862
         15    466.355447
         48    556.091368
         6     641.565693
         26    683.294694
         16    687.194301
         22    696.663817
         45    761.306957
         33    792.380236
         20    844.633515
         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:

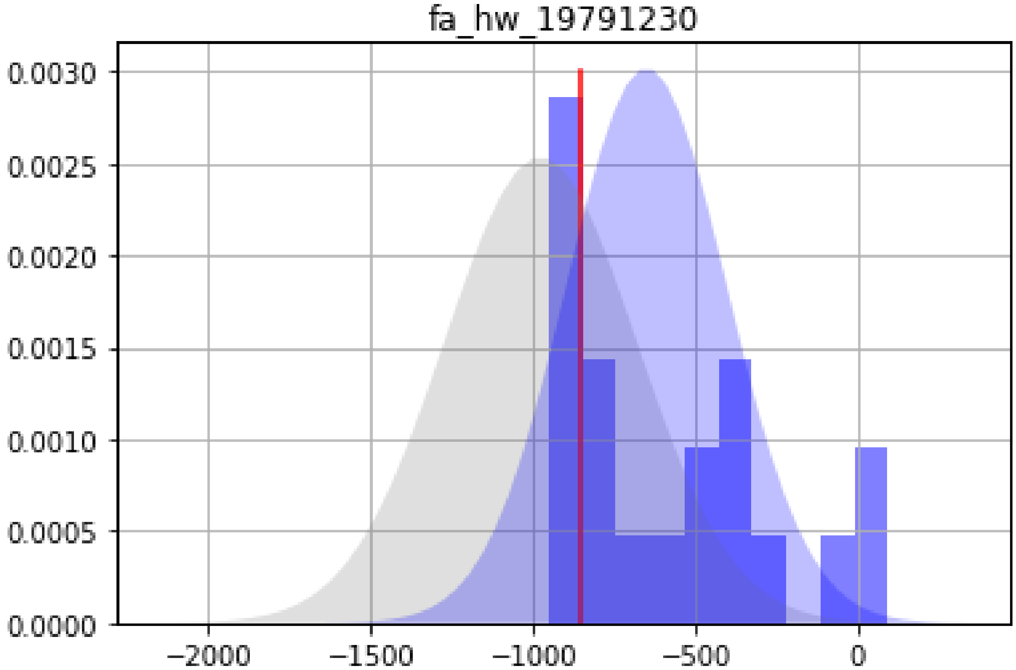
```
In [26]: oe_pt = oe.loc[oe.phi_vector.sort_values().index[:20],:]
```

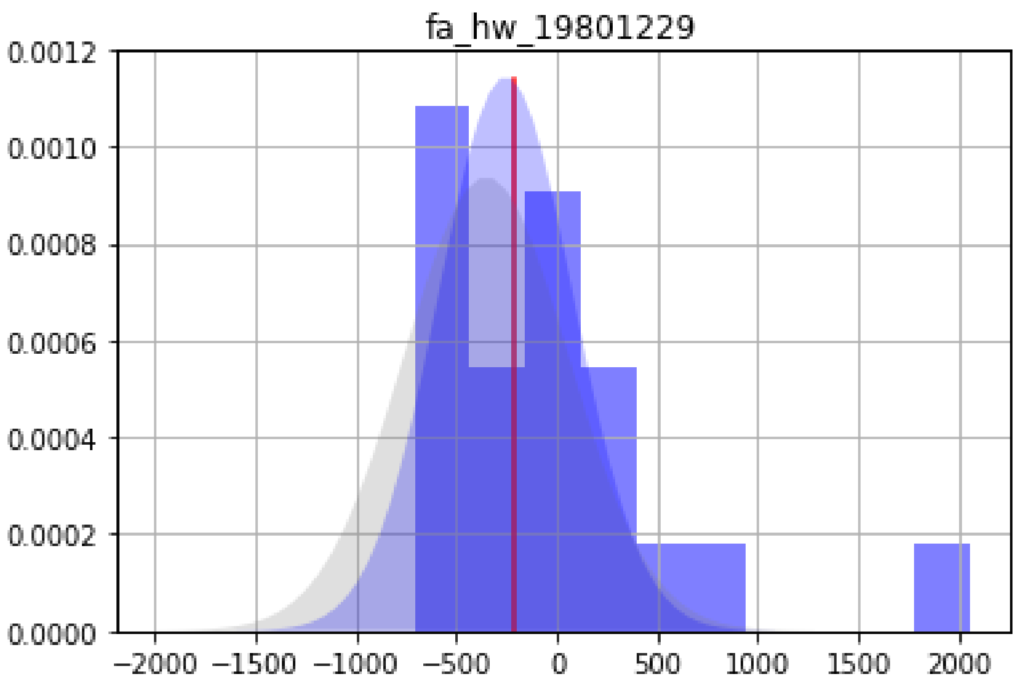
```
In [27]: f_df = pd.read_csv(os.path.join(m_d,"freyberg_pp.pred.usum.csv"),index_col=0)
         f_df.index = f_df.index.map(str.lower)
         f_df
```

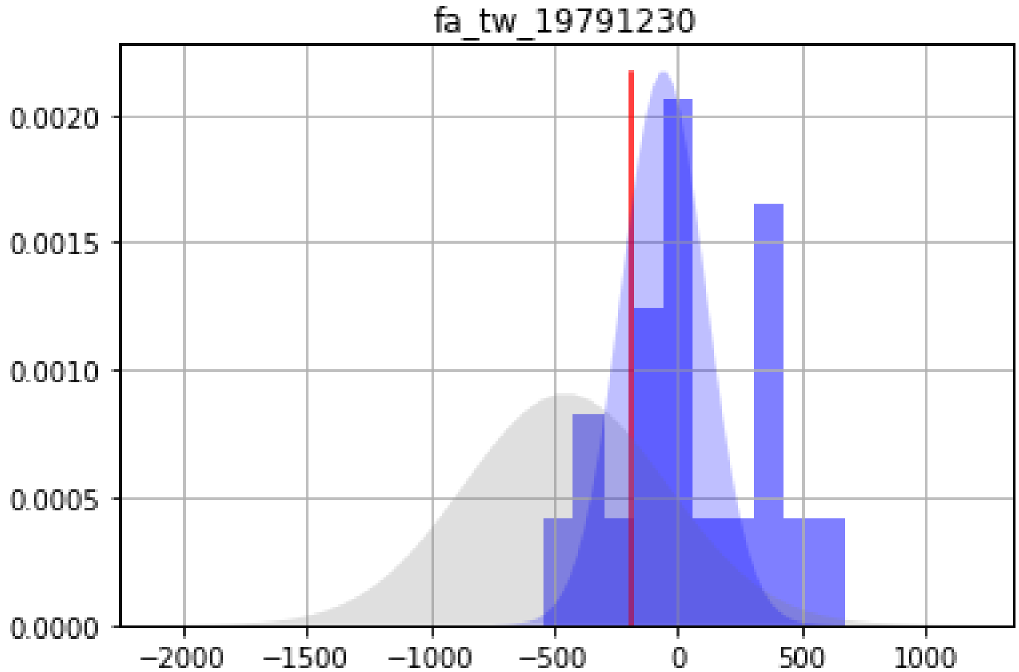
```
Out[27]:                     prior_mean  prior_stdev  prior_lower_bound  \
         name
         fa_hw_19791230       -977.2390    295.32800         -1567.8900
         fa_hw_19801229       -351.2160    409.77000         -1170.7600
         fa_tw_19791230       -453.0330    409.35100         -1271.7400
         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  -650.4570  248.019000
         fa_hw_19801229               468.3240  -254.1730  335.584000
         fa_tw_19791230               365.6690   -57.8134  170.817000
         fa_tw_19801229              1122.4200   279.3360  263.851000
         hds_00_013_002_000            47.5365    39.4960    0.277776
         hds_00_013_002_001            46.4994    38.4735    0.689849
         part_status                    2.0000     2.0000    0.000000
         part_time                   2317.2000  1003.5700  603.650000

                             post_lower_bound  post_upper_bound
         name
         fa_hw_19791230             -1146.5000         -154.4190
         fa_hw_19801229              -925.3410          416.9940
         fa_tw_19791230              -399.4470          283.8200
         fa_tw_19801229              -248.3660          807.0390
         hds_00_013_002_000            38.9405           40.0516
         hds_00_013_002_001            37.0938           39.8532
         part_status                    2.0000            2.0000
         part_time                   -203.7280         2210.8700
```

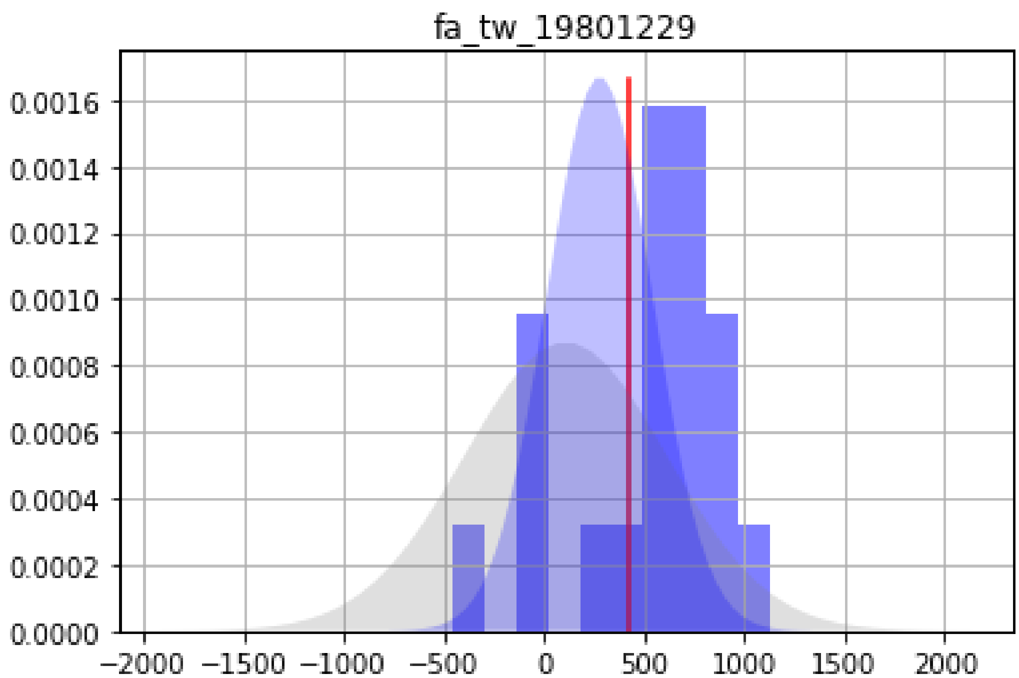
```
In [28]: obs = pst.observation_data
         fnames = pst.pestpp_options["forecasts"].split(",")
         for forecast in fnames:
             ax = plt.subplot(111)
             oe_pt.loc[:,forecast].hist(ax=ax,color="b",alpha=0.5,normed=True)
             ax.plot([obs.loc[forecast,"obsval"],obs.loc[forecast,"obsval"]],ax.get_ylim(),"r"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

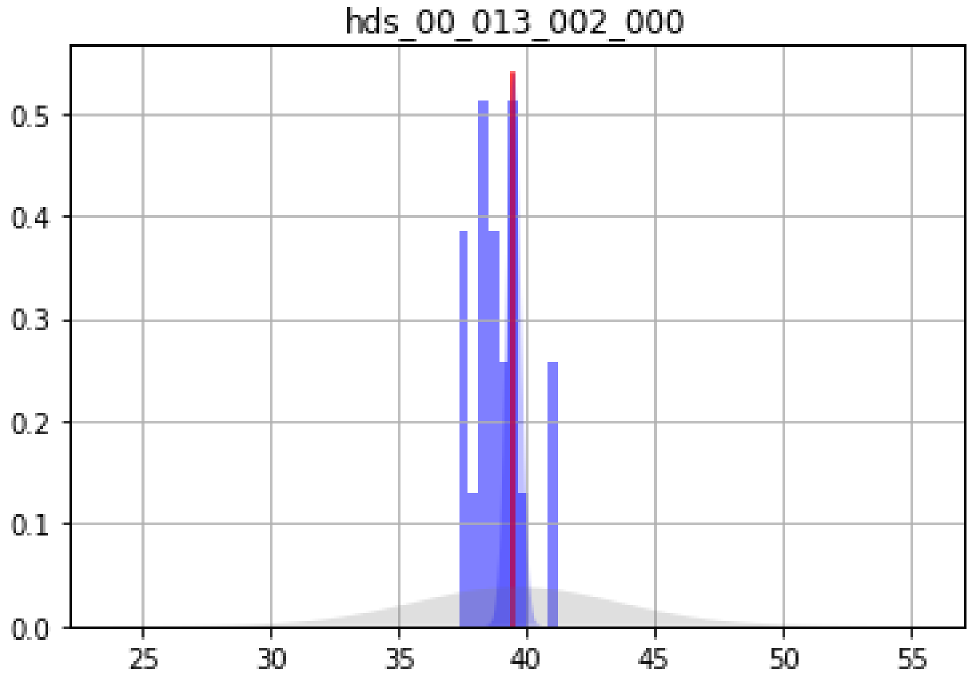
```
axt.set_ylim(0,axt.get_ylim()[1])
axt.set_yticks([])
ax.set_title(forecast)
plt.show()
```

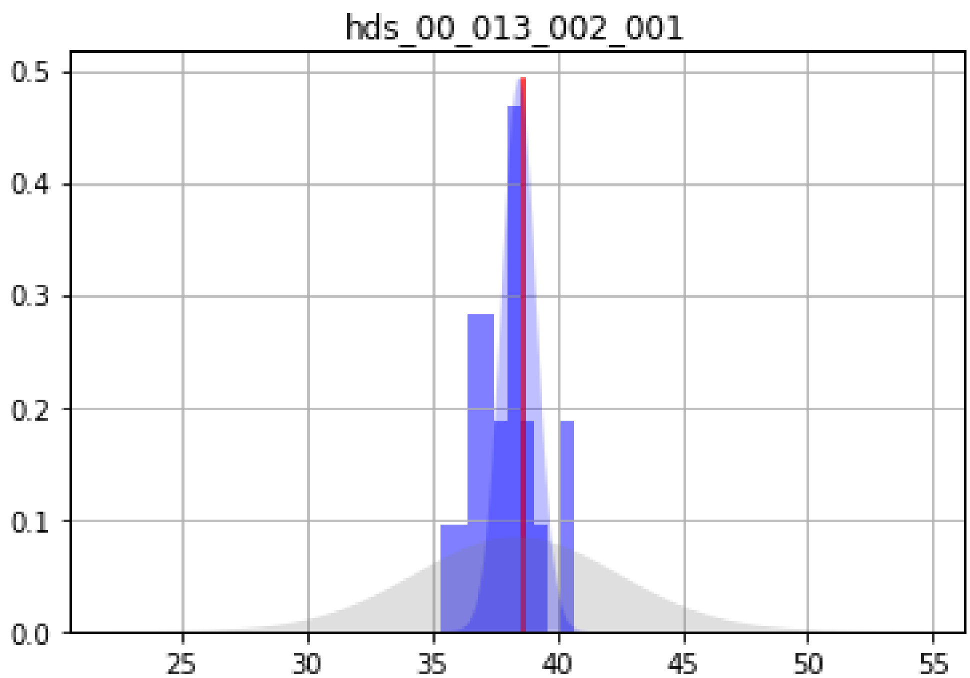


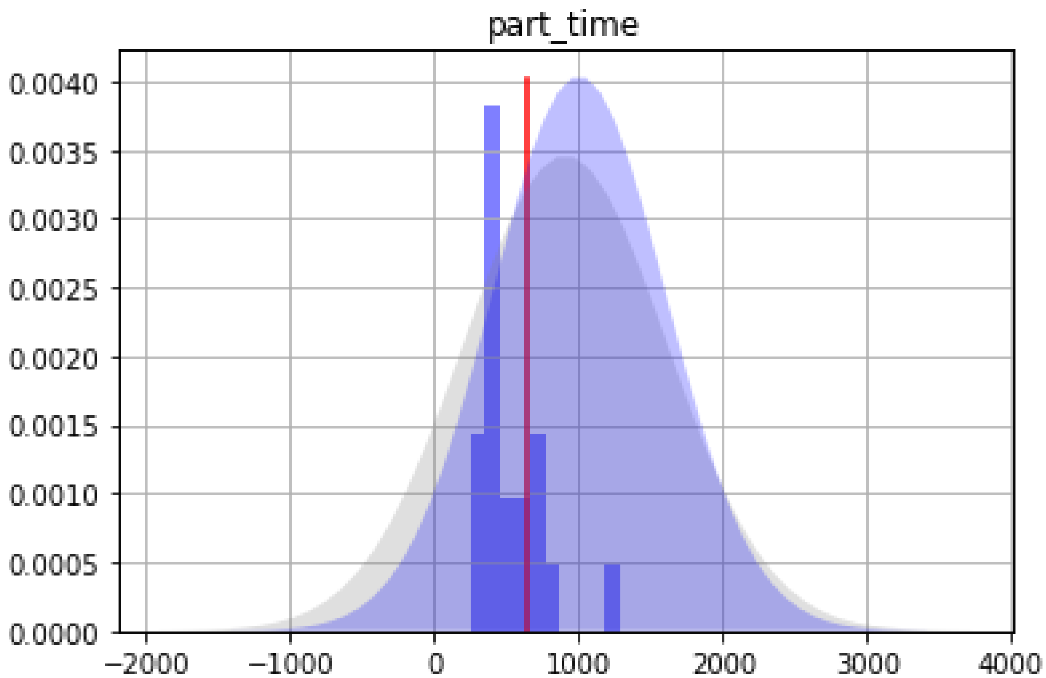


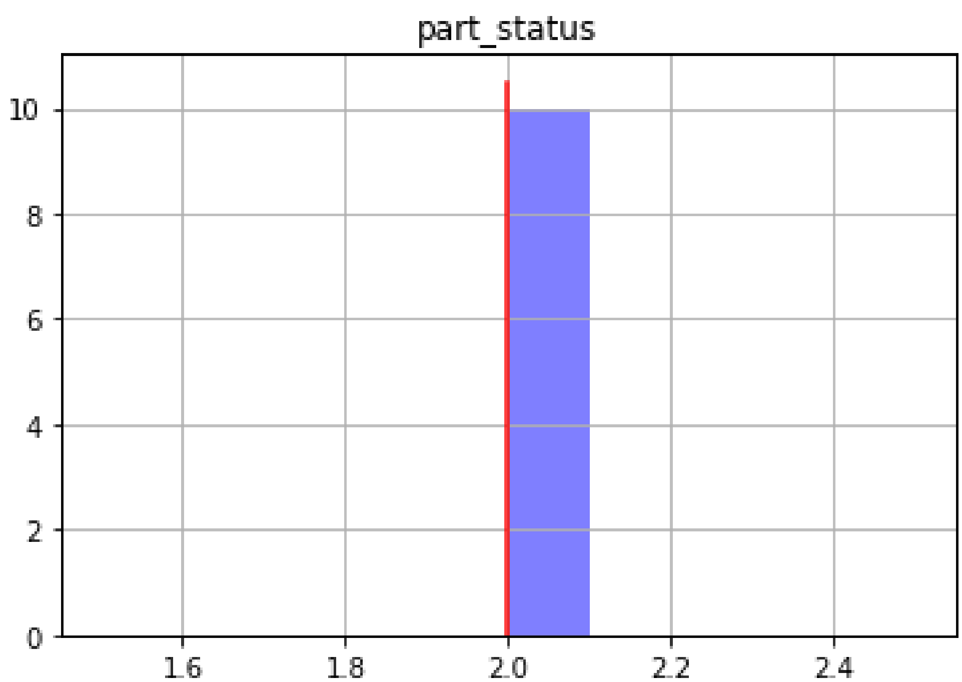

fa_tw_19791230
0.0020
0.0015
0.0010
0.0005
0.0000
−2000
−1500
−1000
−500
0
500
1000


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
25
30
35
40
45
50
55


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


part_time
0.0040
0.0035
0.0030
0.0025
0.0020
0.0015
0.0010
0.0005
0.0000
−2000
−1000
0
1000
2000
3000
4000


part_status
10
8
6
4
2
0
1.6
1.8
2.0
2.2
2.4