pestpp-glm

May 12, 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_vka3           gr_vka3       log    705                  0
        cn_ss8              cn_ss8       log      1                  0
        cn_vka7            cn_vka7       log      1                  0
        gr_hk4              gr_hk4       log    705                  0
        gr_sy4              gr_sy4       log    705                  0
        gr_prsity5    gr_prsity5       log    705                  0
        cn_hk8              cn_hk8       log      1                  0
        gr_vka4            gr_vka4       log    705                  0
        cn_hk7              cn_hk7       log      1                  0
        cn_vka6            cn_vka6       log      1                  0
        cn_prsity8    cn_prsity8       log      1                  0
```

pp_sy0	pp_sy0	log	32	0
gr_sy5	gr_sy5	log	705	0
gr_hk5	gr_hk5	log	705	0
cn_rech5	cn_rech5	log	1	-0.39794
welflux	welflux	log	2	0 to 0.176091
gr_ss3	gr_ss3	log	705	0
pp_rech1	pp_rech1	log	32	0
cn_hk6	cn_hk6	log	1	0
cn_rech4	cn_rech4	log	1	0
pp_vka1	pp_vka1	log	32	0
cn_sy8	cn_sy8	log	1	0
pp_hk1	pp_hk1	log	32	0
pp_hk0	pp_hk0	log	32	0
gr_ss4	gr_ss4	log	705	0
pp_ss1	pp_ss1	log	32	0
pp_prsity1	pp_prsity1	log	32	0
pp_prsity2	pp_prsity2	log	32	0
cn_ss6	cn_ss6	log	1	0
gr_prsity4	gr_prsity4	log	705	0
...	...	...	...	...
gr_vka5	gr_vka5	log	705	0
pp_ss0	pp_ss0	log	32	0
cn_strt8	cn_strt8	log	1	0
gr_ss5	gr_ss5	log	705	0
gr_sy3	gr_sy3	log	705	0
pp_strt0	pp_strt0	log	32	0
cn_prsity7	cn_prsity7	log	1	0
cn_sy6	cn_sy6	log	1	0
strk	strk	log	40	0
flow	flow	log	1	0
cn_strt7	cn_strt7	log	1	0
pp_hk2	pp_hk2	log	32	0
cn_prsity6	cn_prsity6	log	1	0
pp_sy1	pp_sy1	log	32	0
gr_strt3	gr_strt3	log	705	0
pp_sy2	pp_sy2	log	32	0
gr_rech3	gr_rech3	log	705	0
cn_ss7	cn_ss7	log	1	0
pp_ss2	pp_ss2	log	32	0
cn_sy7	cn_sy7	log	1	0
drncond_k00	drncond_k00	log	10	0
gr_strt4	gr_strt4	log	705	0
cn_strt6	cn_strt6	log	1	0
pp_prsity0	pp_prsity0	log	32	0
pp_vka0	pp_vka0	log	32	0
pp_strt2	pp_strt2	log	32	0
cn_vka8	cn_vka8	log	1	0
pp_strt1	pp_strt1	log	32	0

welflux_k02	welflux_k02	log	6	0
pp_rech0	pp_rech0	log	32	0

	upper bound	lower bound	standard deviation
gr_vka3	1	-1	0.5
cn_ss8	1	-1	0.5
cn_vka7	1	-1	0.5
gr_hk4	1	-1	0.5
gr_sy4	0.243038	-0.60206	0.211275
gr_prsity5	0.176091	-0.30103	0.11928
cn_hk8	1	-1	0.5
gr_vka4	1	-1	0.5
cn_hk7	1	-1	0.5
cn_vka6	1	-1	0.5
cn_prsity8	0.176091	-0.30103	0.11928
pp_sy0	0.243038	-0.60206	0.211275
gr_sy5	0.243038	-0.60206	0.211275
gr_hk5	1	-1	0.5
cn_rech5	-0.09691	-1	0.225772
welflux	0.176091 to 0.30103	-0.30103 to 0	0.0752575 to 0.11928
gr_ss3	1	-1	0.5
pp_rech1	0.0413927	-0.0457575	0.0217875
cn_hk6	1	-1	0.5
cn_rech4	0.0791812	-0.09691	0.0440228
pp_vka1	1	-1	0.5
cn_sy8	0.243038	-0.60206	0.211275
pp_hk1	1	-1	0.5
pp_hk0	1	-1	0.5
gr_ss4	1	-1	0.5
pp_ss1	1	-1	0.5
pp_prsity1	0.176091	-0.30103	0.11928
pp_prsity2	0.176091	-0.30103	0.11928
cn_ss6	1	-1	0.5
gr_prsity4	0.176091	-0.30103	0.11928
...	...	...	...
gr_vka5	1	-1	0.5
pp_ss0	1	-1	0.5
cn_strt8	0.0211893	-0.0222764	0.0108664
gr_ss5	1	-1	0.5
gr_sy3	0.243038	-0.60206	0.211275
pp_strt0	0.0211893	-0.0222764	0.0108664
cn_prsity7	0.176091	-0.30103	0.11928
cn_sy6	0.243038	-0.60206	0.211275
strk	2	-2	1
flow	0.09691	-0.124939	0.0554622
cn_strt7	0.0211893	-0.0222764	0.0108664
pp_hk2	1	-1	0.5
cn_prsity6	0.176091	-0.30103	0.11928

```
pp_sy1              0.243038     -0.60206       0.211275
gr_strt3            0.0211893    -0.0222764     0.0108664
pp_sy2              0.243038     -0.60206       0.211275
gr_rech3            0.0413927    -0.0457575     0.0217875
cn_ss7                      1          -1             0.5
pp_ss2                      1          -1             0.5
cn_sy7              0.243038     -0.60206       0.211275
drncond_k00                 1          -1             0.5
gr_strt4            0.0211893    -0.0222764     0.0108664
cn_strt6            0.0211893    -0.0222764     0.0108664
pp_prsity0          0.176091     -0.30103       0.11928
pp_vka0                     1          -1             0.5
pp_strt2            0.0211893    -0.0222764     0.0108664
cn_vka8                     1          -1             0.5
pp_strt1            0.0211893    -0.0222764     0.0108664
welflux_k02                 1          -1             0.5
pp_rech0            0.0413927    -0.0457575     0.0217875

[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_hk8          1
cn_vka8         1
cn_vka7         1
cn_hk6          1
cn_ss8          1
cn_rech5        1
cn_prsity8      1
cn_vka6         1
cn_rech4        1
cn_ss6          1
cn_ss7          1
cn_strt8        1
cn_hk7          1
cn_prsity7      1
cn_sy6          1
flow            1
cn_strt7        1
cn_prsity6      1
cn_sy7          1
cn_strt6        1
welflux         2
welflux_k02     6
drncond_k00    10
pp_vka0        32
pp_ss0         32
pp_hk2         32
pp_hk1         32
pp_hk0         32
pp_ss1         32
pp_prsity1     32
pp_prsity2     32
pp_vka2        32
pp_rech1       32
pp_strt0       32
pp_rech0       32
pp_vka1        32
pp_prsity0     32
```

```
pp_sy1         32
pp_sy2         32
pp_ss2         32
pp_strt1       32
pp_strt2       32
pp_sy0         32
strk           40
Name: pargp, dtype: int64
```

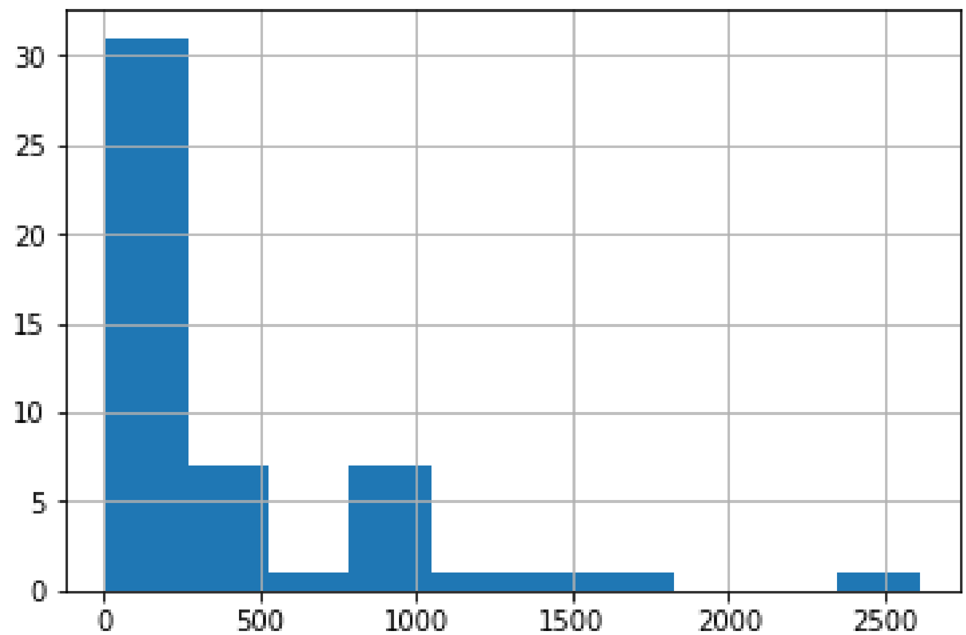
fix the future recharge pilot points, vka in layers 1 and 3 and the initial condition pilot points (we still have layer-scale pars for each of these types)

```
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"))

noptmax:3, npar_adj:527, nnz_obs:14


In [12]: pyemu.os_utils.start_slaves(t_d,"pestpp-glm","freyberg_pp.pst",num_slaves=20,slave_roo
                                     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
         47     5.930917
         23     9.276885
         48    12.105952
         26    13.318840
         12    14.758830
         44    15.693285
```

```
38    16.297832
21    16.626313
5     18.763521
10    19.877588
11    21.870993
29    25.867738
9     29.485384
7     35.392319
39    42.190815
45    49.462404
24    51.648284
1     52.957698
41    57.181593
33    62.171324
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:

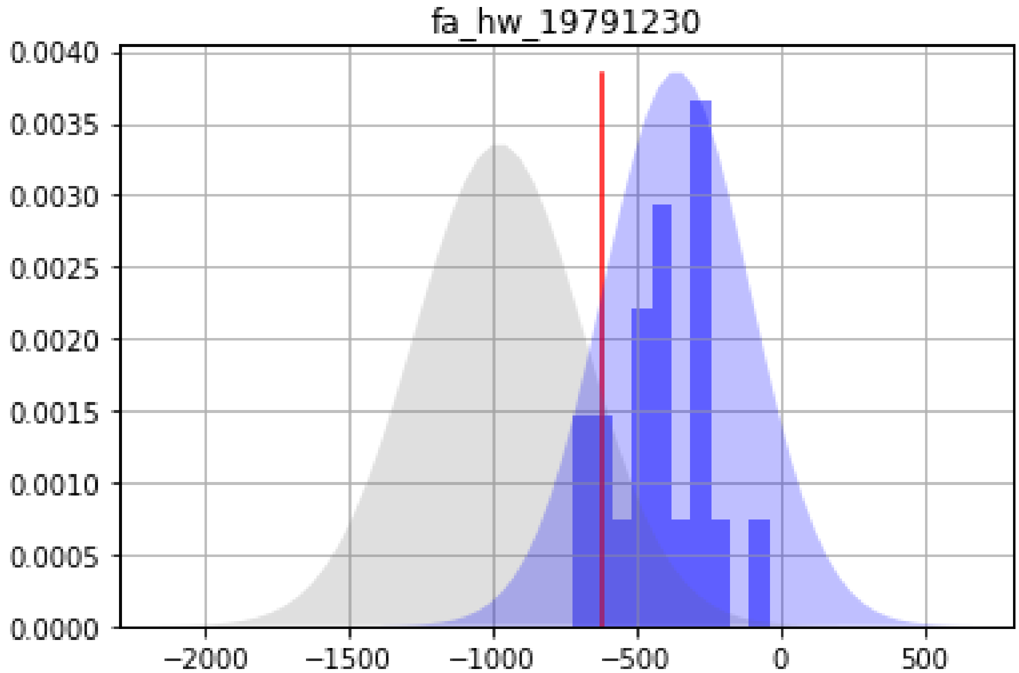
```
In [15]: oe_pt = oe.loc[oe.phi_vector.sort_values().index[:20],:] #just take the 20 lowest phi
```

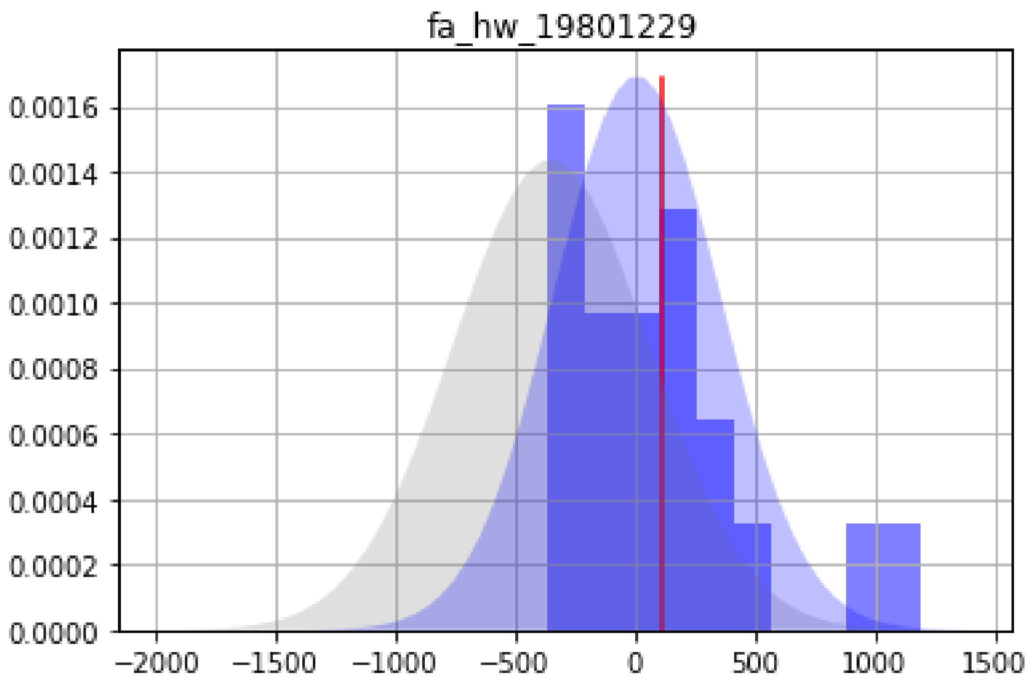
We can also load and plot the FOSM forecast results along side of the ensemble results:

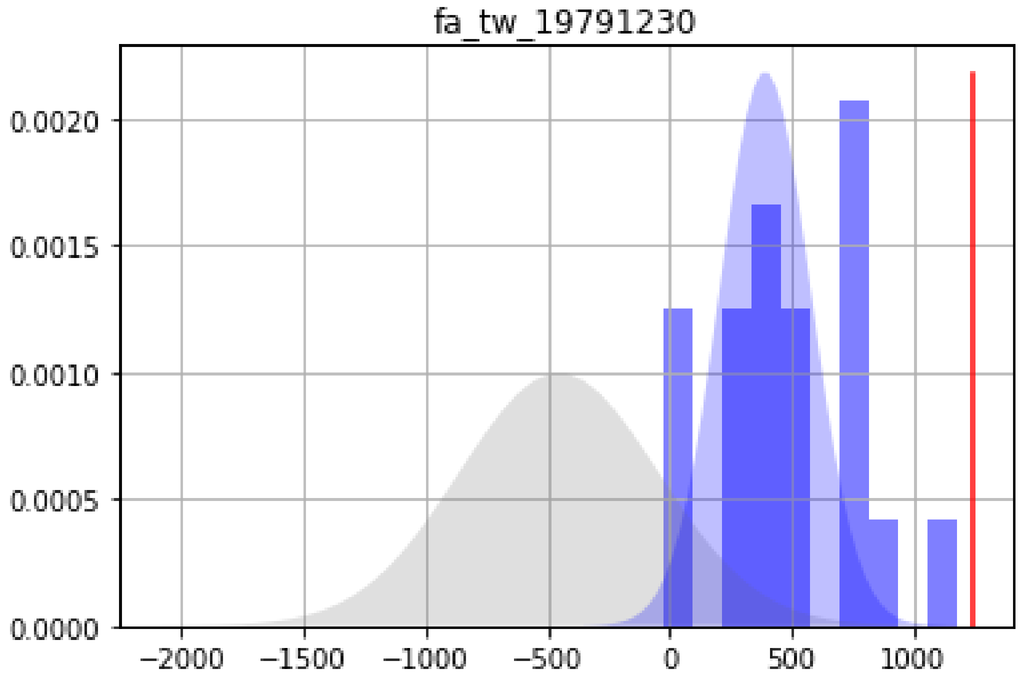
```
In [16]: f_df = pd.read_csv(os.path.join(m_d,"freyberg_pp.pred.usum.csv"),index_col=0)
         f_df.index = f_df.index.map(str.lower)
         f_df
```

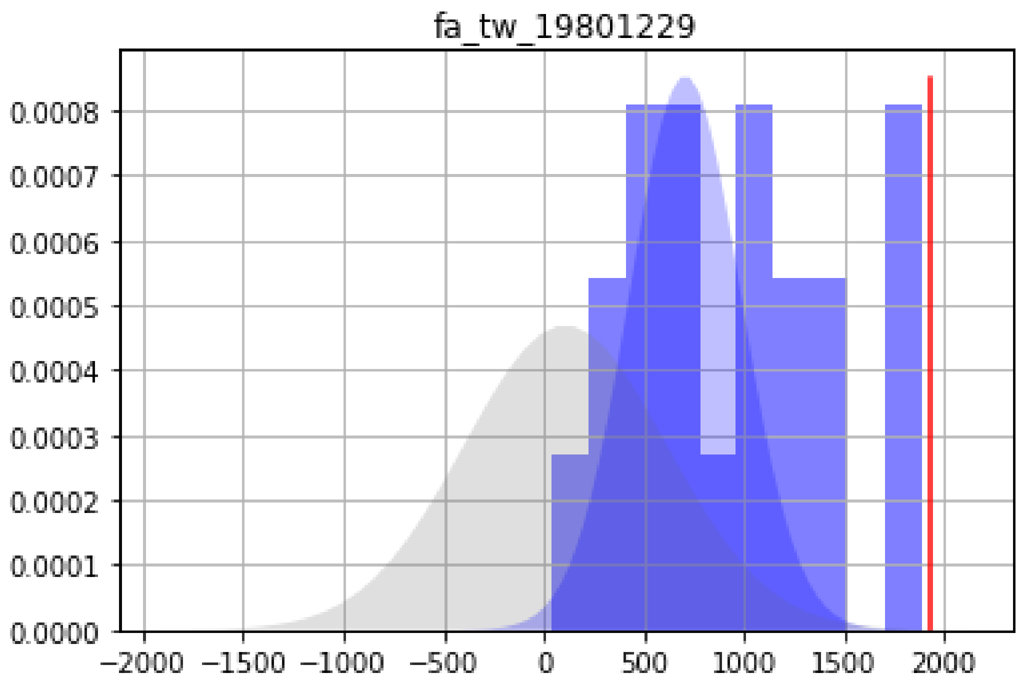
Out[16]:
```
                     prior_mean  prior_stdev  prior_lower_bound  \
name
fa_hw_19791230        -977.2390    295.32800         -1567.8900
fa_hw_19801229        -351.2160    409.77000         -1170.7600
fa_tw_19791230        -453.0330    409.35100         -1271.7400
fa_tw_19801229         108.9600    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    570.98600          -234.2690

                     prior_upper_bound  post_mean  post_stdev  \
name
fa_hw_19791230               -386.5840  -359.9670  256.719000
fa_hw_19801229                468.3240     7.9574  347.960000
fa_tw_19791230                365.6690   393.0230  186.659000
fa_tw_19801229               1122.4200   707.6210  278.383000
hds_00_013_002_000             47.5365    35.8677    0.377760
hds_00_013_002_001             46.4994    35.2034    0.734614
part_status                     2.0000     2.0000    0.000000
part_time                    2049.6700   611.9380  443.232000

                     post_lower_bound  post_upper_bound
name
fa_hw_19791230              -873.4050          153.4710
fa_hw_19801229              -687.9620          703.8770
fa_tw_19791230                19.7049          766.3410
fa_tw_19801229               150.8550         1264.3900
hds_00_013_002_000            35.1122           36.6232
hds_00_013_002_001            33.7341           36.6726
part_status                    2.0000            2.0000
part_time                   -274.5260         1498.4000
```

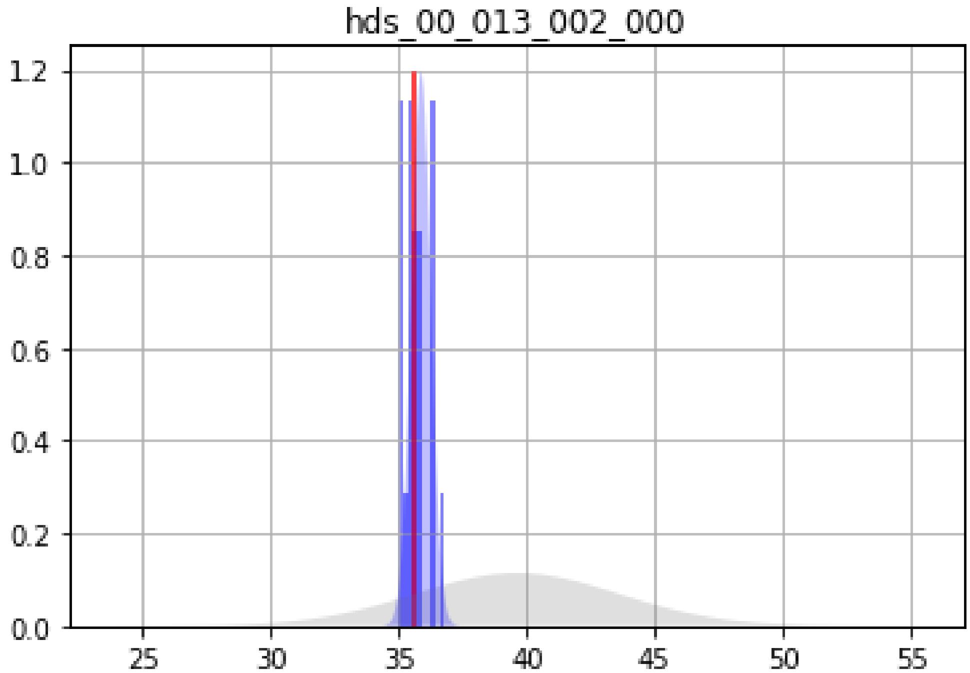
In [17]:
```
obs = pst.observation_data
fnames = pst.pestpp_options["forecasts"].split(",")
for forecast in fnames:
    ax = plt.subplot(111)
    oe_pt.loc[:,forecast].hist(ax=ax,color="b",alpha=0.5,normed=True)
    ax.plot([obs.loc[forecast,"obsval"],obs.loc[forecast,"obsval"]],ax.get_ylim(),"r"
  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

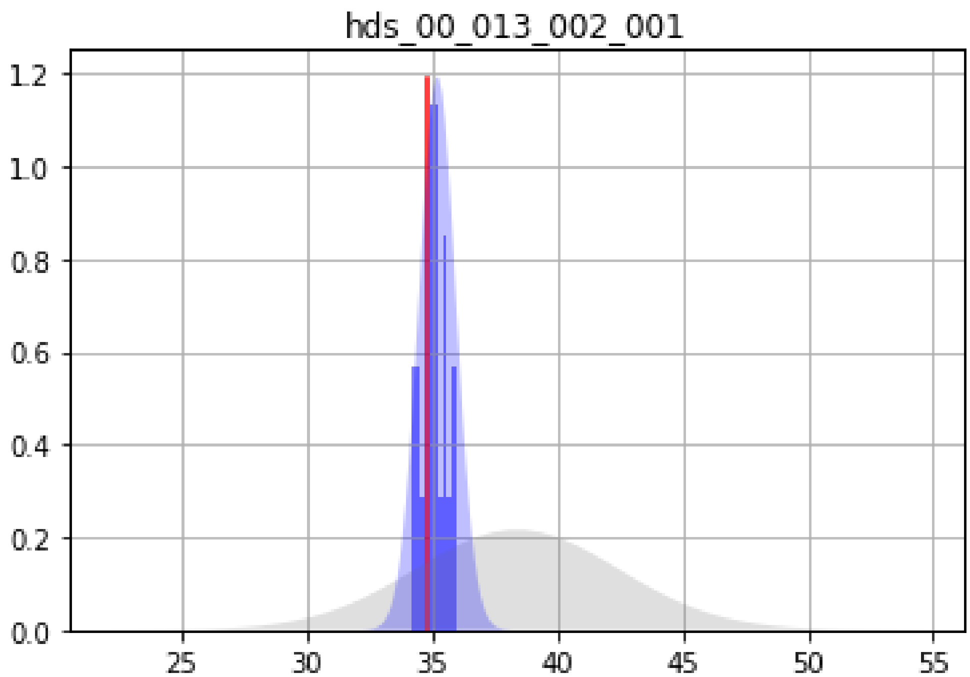

fa_hw_19791230
0.0040
0.0035
0.0030
0.0025
0.0020
0.0015
0.0010
0.0005
0.0000
−2000
−1500
−1000
−500
0
500

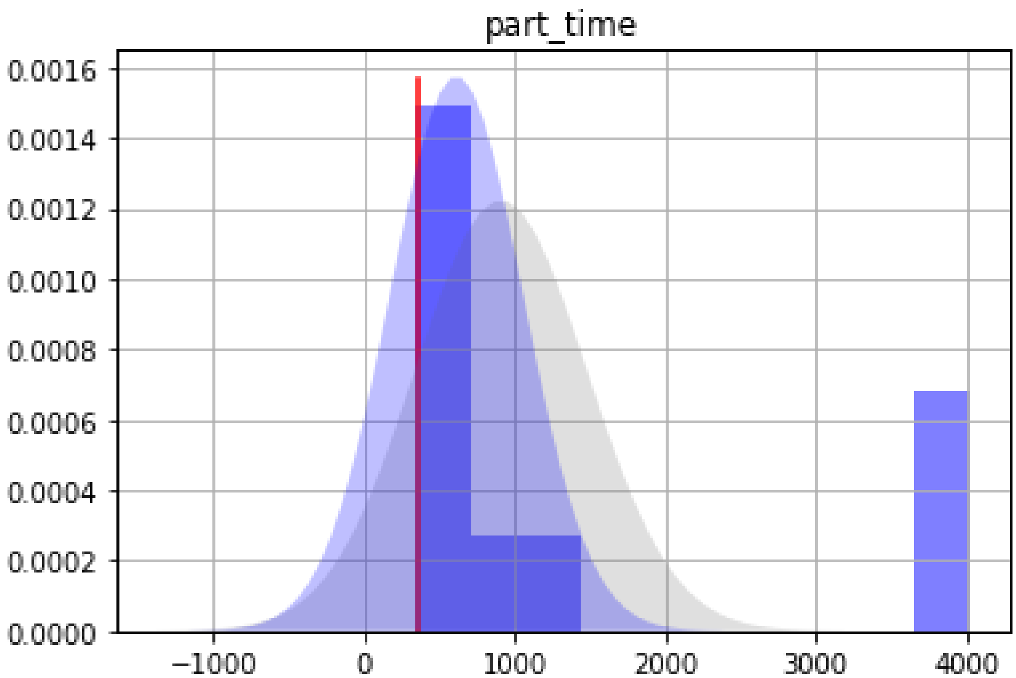

fa_hw_19801229
0.0016
0.0014
0.0012
0.0010
0.0008
0.0006
0.0004
0.0002
0.0000
−2000
−1500
−1000
−500
0
500
1000
1500

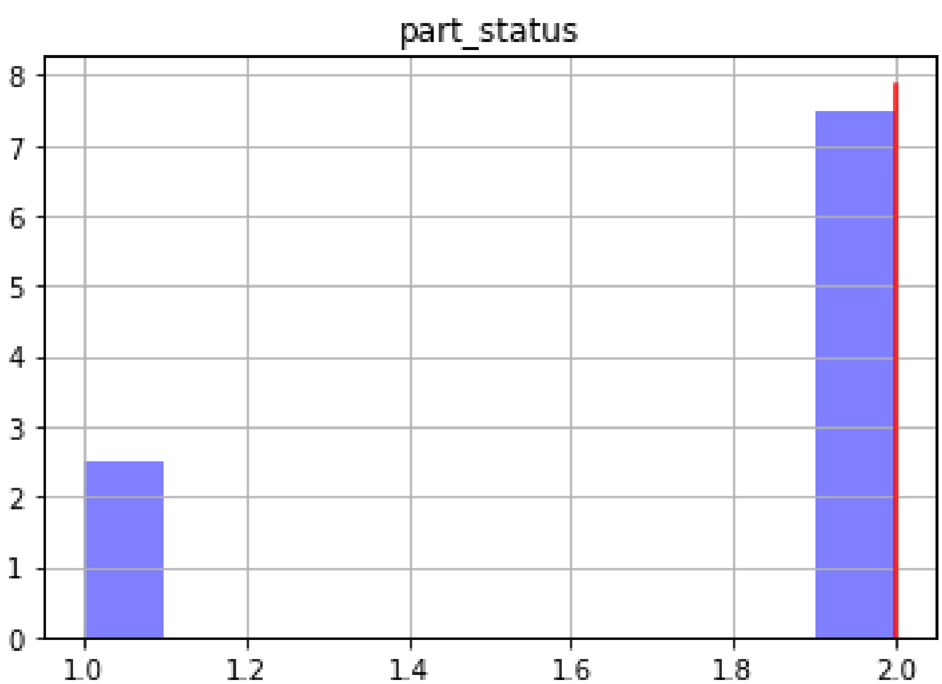

fa_tw_19791230
0.0020
0.0015
0.0010
0.0005
0.0000
−2000
−1500
−1000
−500
0
500
1000


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
1.2
1.0
0.8
0.6
0.4
0.2
0.0
25
30
35
40
45
50
55


hds_00_013_002_001
1.2
1.0
0.8
0.6
0.4
0.2
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
−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"))
```

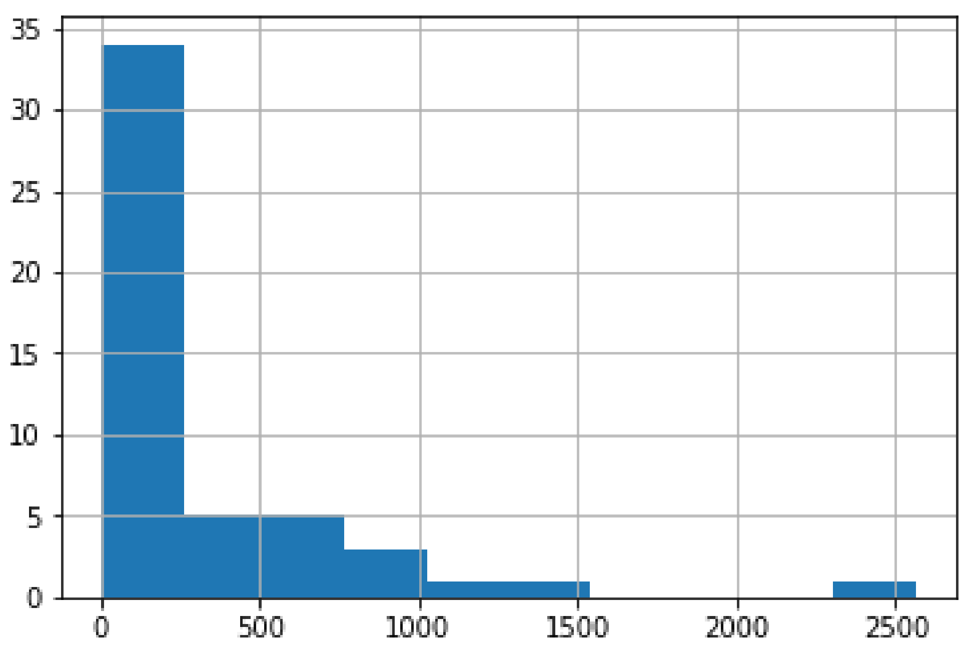
```
noptmax:3, npar_adj:527, nnz_obs:14
```

```
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
5      4.663889
48     7.684285
38     8.298100
23     8.534114
47     9.583777
21    11.620879
10    12.520142
17    13.616306
24    19.101539
11    20.349773
1     22.283044
44    23.480130
35    25.509411
26    31.412505
39    32.871846
41    32.971337
12    34.458375
6     52.946592
9     55.913683
29    57.536024
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]:

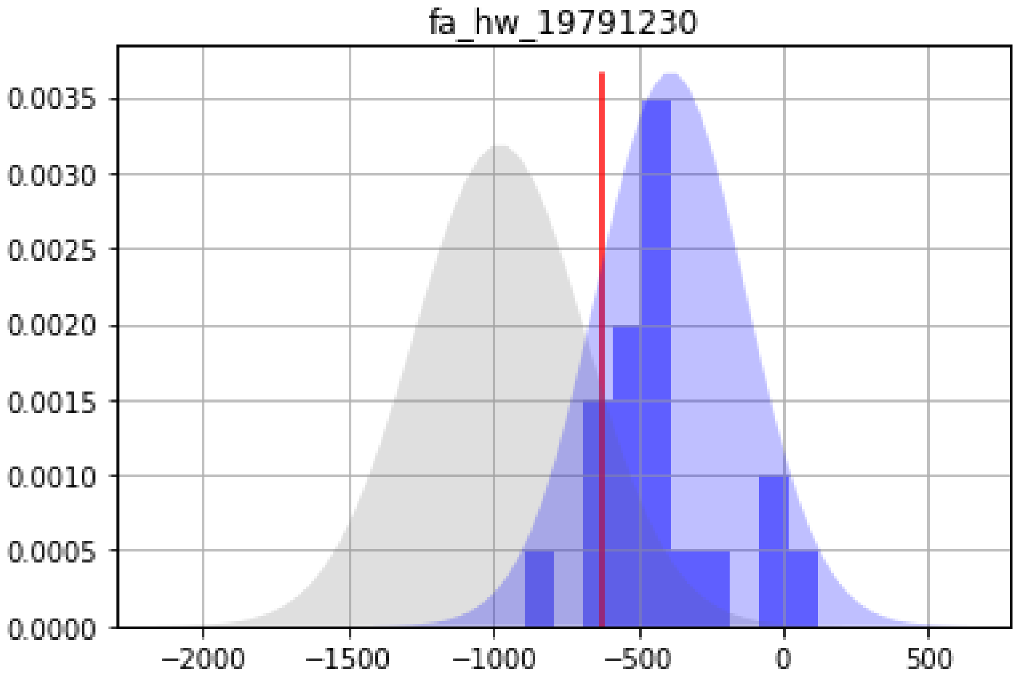
name	prior_mean	prior_stdev	prior_lower_bound
fa_hw_19791230	-977.2390	295.32800	-1567.8900
fa_hw_19801229	-351.2160	409.77000	-1170.7600
fa_tw_19791230	-453.0330	409.35100	-1271.7400
fa_tw_19801229	108.9600	506.73200	-904.5040
hds_00_013_002_000	39.6102	3.96314	31.6840
hds_00_013_002_001	38.3838	4.05782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

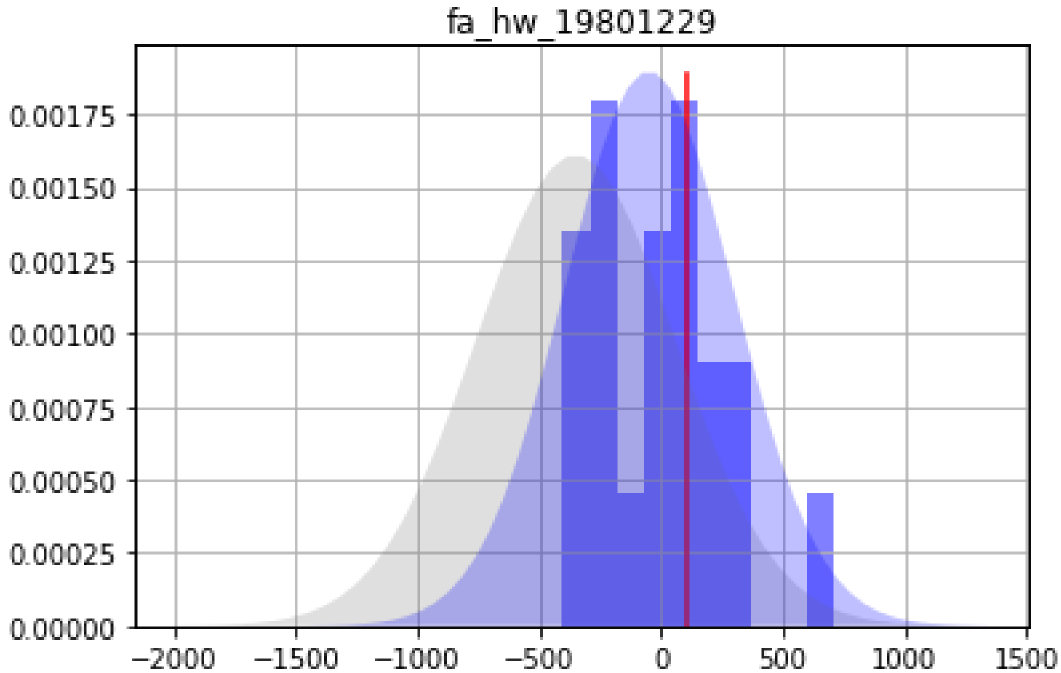
name	prior_upper_bound	post_mean	post_stdev
fa_hw_19791230	-386.5840	-387.1910	256.744000
fa_hw_19801229	468.3240	-50.5100	347.977000
fa_tw_19791230	365.6690	267.9340	186.813000
fa_tw_19801229	1122.4200	560.0230	278.412000
hds_00_013_002_000	47.5365	36.2226	0.411703
hds_00_013_002_001	46.4994	35.5583	0.752386
part_status	2.0000	2.0000	0.000000
part_time	2049.6700	883.6440	445.017000

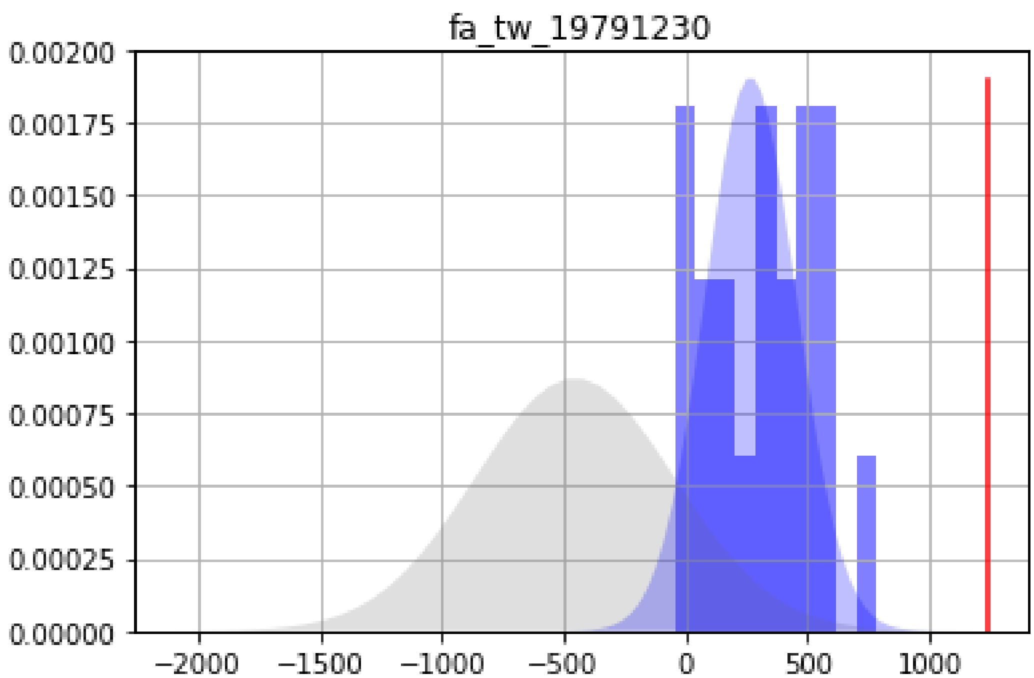
name	post_lower_bound	post_upper_bound
fa_hw_19791230	-900.68000	126.2970
fa_hw_19801229	-746.46300	645.4430
fa_tw_19791230	-105.69100	641.5600
fa_tw_19801229	3.19948	1116.8500
hds_00_013_002_000	35.39920	37.0460
hds_00_013_002_001	34.05350	37.0631
part_status	2.00000	2.0000
part_time	-6.38939	1773.6800

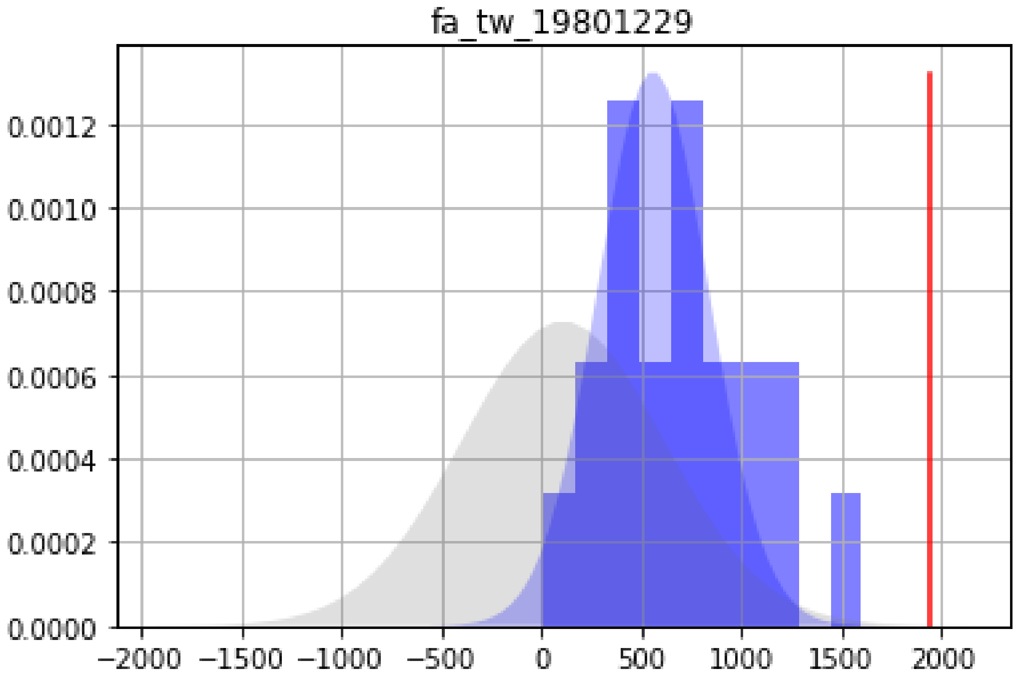
```
In [28]: obs = pst.observation_data
         fnames = pst.pestpp_options["forecasts"].split(",")
         for forecast in fnames:
             ax = plt.subplot(111)
             oe_pt.loc[:,forecast].hist(ax=ax,color="b",alpha=0.5,normed=True)
             ax.plot([obs.loc[forecast,"obsval"],obs.loc[forecast,"obsval"]],ax.get_ylim(),"r"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

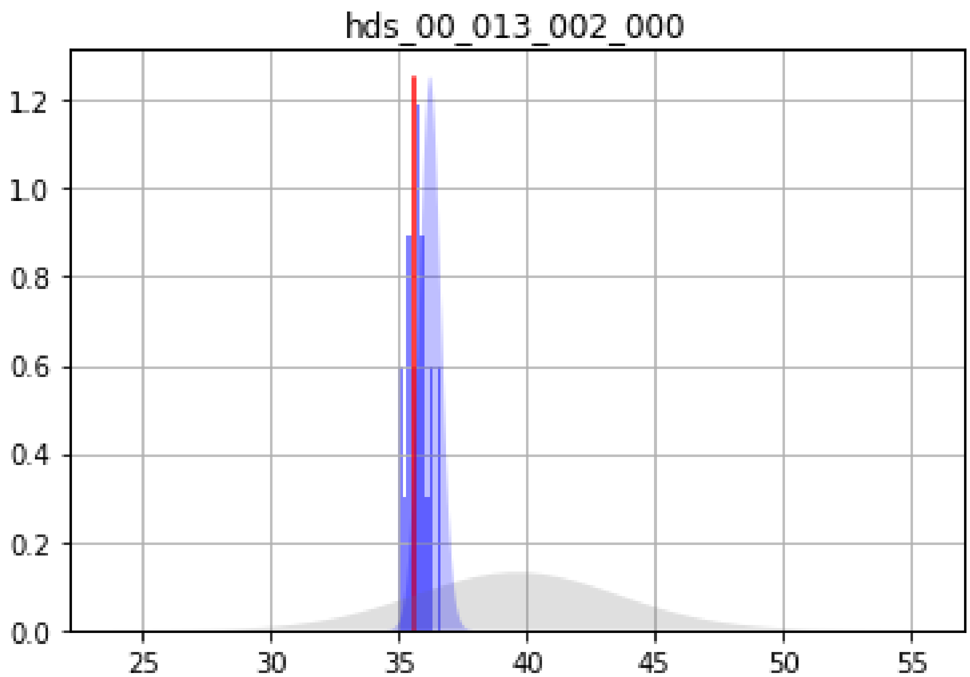
```
x,y = pyemu.plot_utils.gaussian_distribution(f_df.loc[forecast,"prior_mean"],f_df
axt.fill_between(x,0,y,facecolor="0.5",alpha=0.25)
x,y = pyemu.plot_utils.gaussian_distribution(f_df.loc[forecast,"post_mean"],f_df.l
axt.fill_between(x,0,y,facecolor="b",alpha=0.25)
axt.set_ylim(0,axt.get_ylim()[1])
axt.set_yticks([])
ax.set_title(forecast)
plt.show()
```

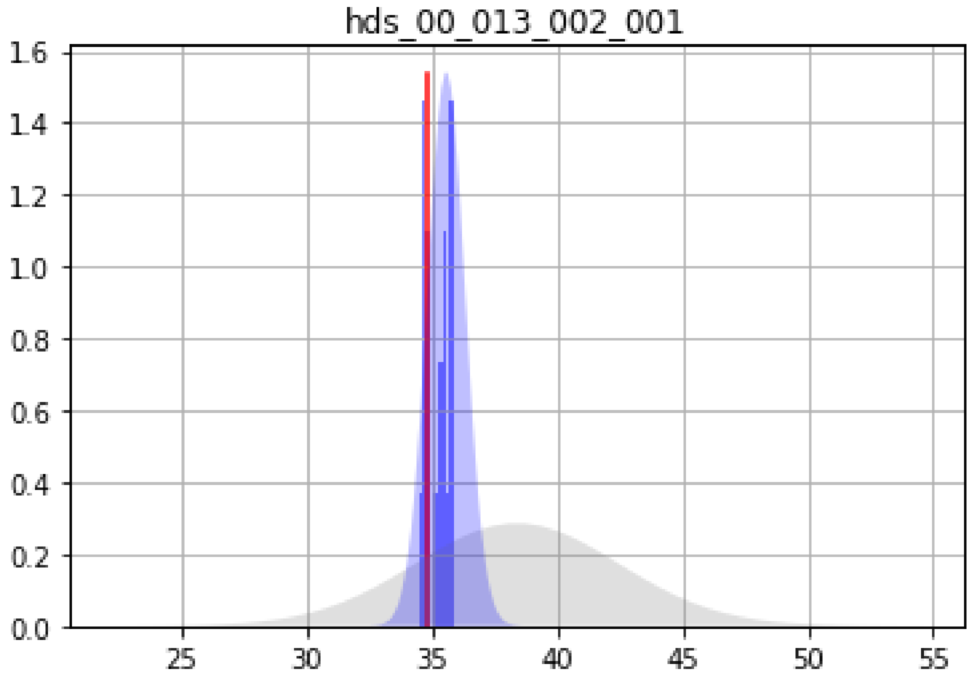


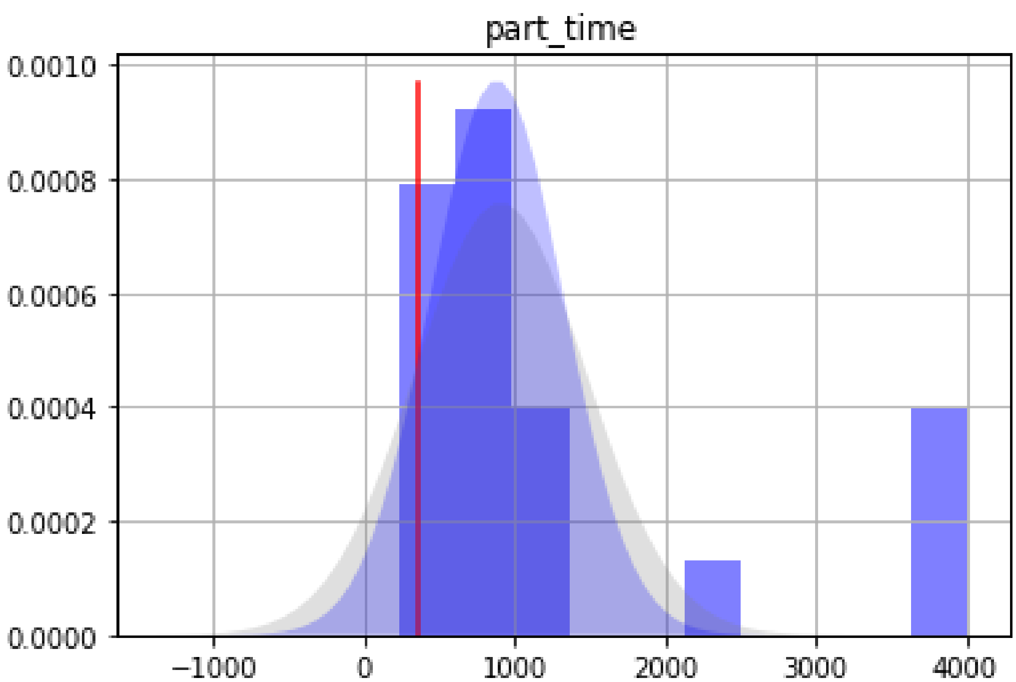

fa_hw_19801229
0.00175
0.00150
0.00125
0.00100
0.00075
0.00050
0.00025
0.00000
−2000
−1500
−1000
−500
0
500
1000
1500

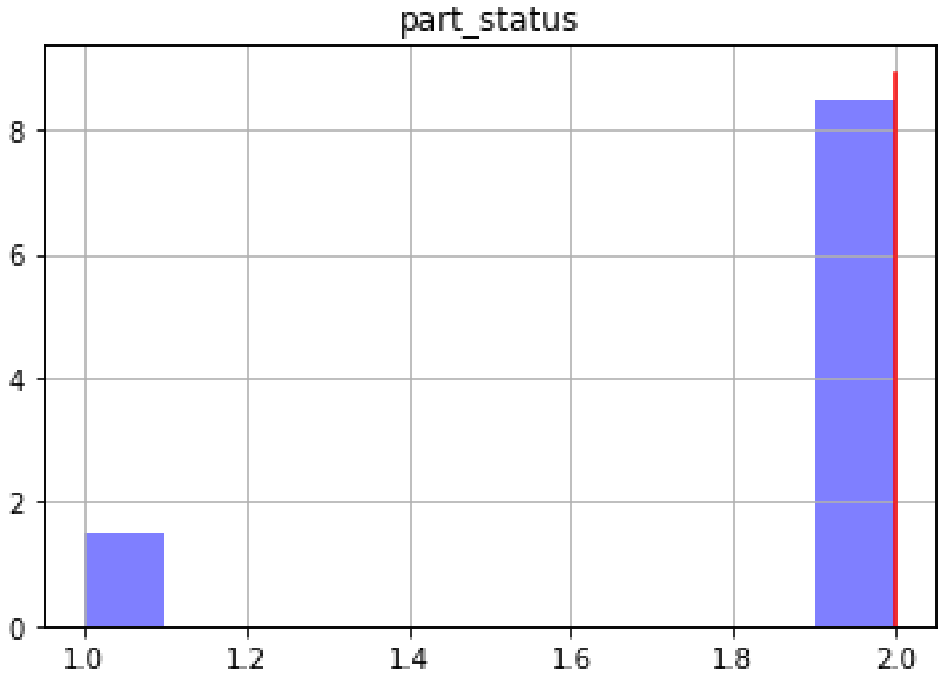

fa_tw_19791230
0.00200
0.00175
0.00150
0.00125
0.00100
0.00075
0.00050
0.00025
0.00000
−2000
−1500
−1000
−500
0
500
1000


fa_tw_19801229
0.0012
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
1.2
1.0
0.8
0.6
0.4
0.2
0.0
25
30
35
40
45
50
55


hds_00_013_002_001
1.6
1.4
1.2
1.0
0.8
0.6
0.4
0.2
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