pestpp-glm

May 8, 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	upper bound \
gr_prsity4	gr_prsity4	log	705	0	0.176091
cn_ss7	cn_ss7	log	1	0	1
gr_prsity3	gr_prsity3	log	705	0	0.176091
gr_prsity5	gr_prsity5	log	705	0	0.176091
cn_rech5	cn_rech5	log	1	-0.39794	-0.09691
cn_hk8	cn_hk8	log	1	0	1
gr_sy5	gr_sy5	log	705	0	0.243038
gr_rech2	gr_rech2	log	705	0	0.0413927
cn_strt6	cn_strt6	log	1	0	0.0211893
gr_ss4	gr_ss4	log	705	0	1
cn_vka6	cn_vka6	log	1	0	1

gr_vka3	gr_vka3	log	705	0	1
pp_sy0	pp_sy0	log	32	0	0.243038
pp_prsity0	pp_prsity0	log	32	0	0.176091
pp_prsity1	pp_prsity1	log	32	0	0.176091
cn_ss6	cn_ss6	log	1	0	1
gr_ss5	gr_ss5	log	705	0	1
cn_prsity6	cn_prsity6	log	1	0	0.176091
flow	flow	log	1	0	0.09691
pp_ss2	pp_ss2	log	32	0	1
cn_sy6	cn_sy6	log	1	0	0.243038
cn_strt7	cn_strt7	log	1	0	0.0211893
gr_rech3	gr_rech3	log	705	0	0.0413927
pp_hk2	pp_hk2	log	32	0	1
gr_sy4	gr_sy4	log	705	0	0.243038
pp_strt2	pp_strt2	log	32	0	0.0211893
gr_hk3	gr_hk3	log	705	0	1
cn_vka7	cn_vka7	log	1	0	1
pp_strt1	pp_strt1	log	32	0	0.0211893
cn_strt8	cn_strt8	log	1	0	0.0211893
...	...	...	...	...	...
gr_strt3	gr_strt3	log	705	0	0.0211893
gr_hk5	gr_hk5	log	705	0	1
pp_rech1	pp_rech1	log	32	0	0.0413927
pp_hk1	pp_hk1	log	32	0	1
pp_sy1	pp_sy1	log	32	0	0.243038
gr_strt5	gr_strt5	log	705	0	0.0211893
welflux_k02	welflux_k02	log	6	0	1
pp_ss0	pp_ss0	log	32	0	1
cn_prsity8	cn_prsity8	log	1	0	0.176091
pp_rech0	pp_rech0	log	32	0	0.0413927
gr_hk4	gr_hk4	log	705	0	1
cn_sy7	cn_sy7	log	1	0	0.243038
gr_sy3	gr_sy3	log	705	0	0.243038
pp_strt0	pp_strt0	log	32	0	0.0211893
drncond_k00	drncond_k00	log	10	0	1
cn_hk7	cn_hk7	log	1	0	1
pp_vka0	pp_vka0	log	32	0	1
cn_ss8	cn_ss8	log	1	0	1
cn_prsity7	cn_prsity7	log	1	0	0.176091
gr_ss3	gr_ss3	log	705	0	1
pp_hk0	pp_hk0	log	32	0	1
cn_vka8	cn_vka8	log	1	0	1
pp_prsity2	pp_prsity2	log	32	0	0.176091
pp_vka2	pp_vka2	log	32	0	1
cn_rech4	cn_rech4	log	1	0	0.0791812
cn_sy8	cn_sy8	log	1	0	0.243038
gr_strt4	gr_strt4	log	705	0	0.0211893
gr_vka4	gr_vka4	log	705	0	1

pp_vka1	pp_vka1	log	32	0	1
pp_ss1	pp_ss1	log	32	0	1

	lower bound	standard deviation
gr_prsity4	-0.30103	0.11928
cn_ss7	-1	0.5
gr_prsity3	-0.30103	0.11928
gr_prsity5	-0.30103	0.11928
cn_rech5	-1	0.225772
cn_hk8	-1	0.5
gr_sy5	-0.60206	0.211275
gr_rech2	-0.0457575	0.0217875
cn_strt6	-0.0222764	0.0108664
gr_ss4	-1	0.5
cn_vka6	-1	0.5
gr_vka3	-1	0.5
pp_sy0	-0.60206	0.211275
pp_prsity0	-0.30103	0.11928
pp_prsity1	-0.30103	0.11928
cn_ss6	-1	0.5
gr_ss5	-1	0.5
cn_prsity6	-0.30103	0.11928
flow	-0.124939	0.0554622
pp_ss2	-1	0.5
cn_sy6	-0.60206	0.211275
cn_strt7	-0.0222764	0.0108664
gr_rech3	-0.0457575	0.0217875
pp_hk2	-1	0.5
gr_sy4	-0.60206	0.211275
pp_strt2	-0.0222764	0.0108664
gr_hk3	-1	0.5
cn_vka7	-1	0.5
pp_strt1	-0.0222764	0.0108664
cn_strt8	-0.0222764	0.0108664
...	...	...
gr_strt3	-0.0222764	0.0108664
gr_hk5	-1	0.5
pp_rech1	-0.0457575	0.0217875
pp_hk1	-1	0.5
pp_sy1	-0.60206	0.211275
gr_strt5	-0.0222764	0.0108664
welflux_k02	-1	0.5
pp_ss0	-1	0.5
cn_prsity8	-0.30103	0.11928
pp_rech0	-0.0457575	0.0217875
gr_hk4	-1	0.5
cn_sy7	-0.60206	0.211275
gr_sy3	-0.60206	0.211275

```
pp_strt0      -0.0222764           0.0108664
drncond_k00           -1                 0.5
cn_hk7                -1                 0.5
pp_vka0               -1                 0.5
cn_ss8                -1                 0.5
cn_prsity7      -0.30103             0.11928
gr_ss3                -1                 0.5
pp_hk0                -1                 0.5
cn_vka8               -1                 0.5
pp_prsity2      -0.30103             0.11928
pp_vka2               -1                 0.5
cn_rech4        -0.09691           0.0440228
cn_sy8          -0.60206            0.211275
gr_strt4      -0.0222764           0.0108664
gr_vka4               -1                 0.5
pp_vka1               -1                 0.5
pp_ss1                -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_ss7           1
cn_hk8           1
cn_rech5         1
cn_strt6         1
cn_vka6          1
cn_ss6           1
cn_prsity6       1
cn_sy7           1
flow             1
cn_hk6           1
cn_strt7         1
cn_vka7          1
cn_strt8         1
cn_rech4         1
cn_prsity8       1
cn_hk7           1
cn_ss8           1
cn_vka8          1
cn_sy8           1
cn_prsity7       1
cn_sy6           1
welflux          2
welflux_k02      6
drncond_k00     10
pp_vka0         32
pp_ss1          32
pp_strt0        32
pp_hk2          32
pp_strt2        32
pp_strt1        32
pp_sy2          32
pp_vka1         32
pp_rech1        32
pp_hk1          32
pp_prsity1      32
pp_ss2          32
pp_rech0        32
pp_prsity0      32
```

```
pp_hk0         32
pp_sy0         32
pp_vka2        32
pp_prsity2     32
pp_sy1         32
pp_ss0         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
```

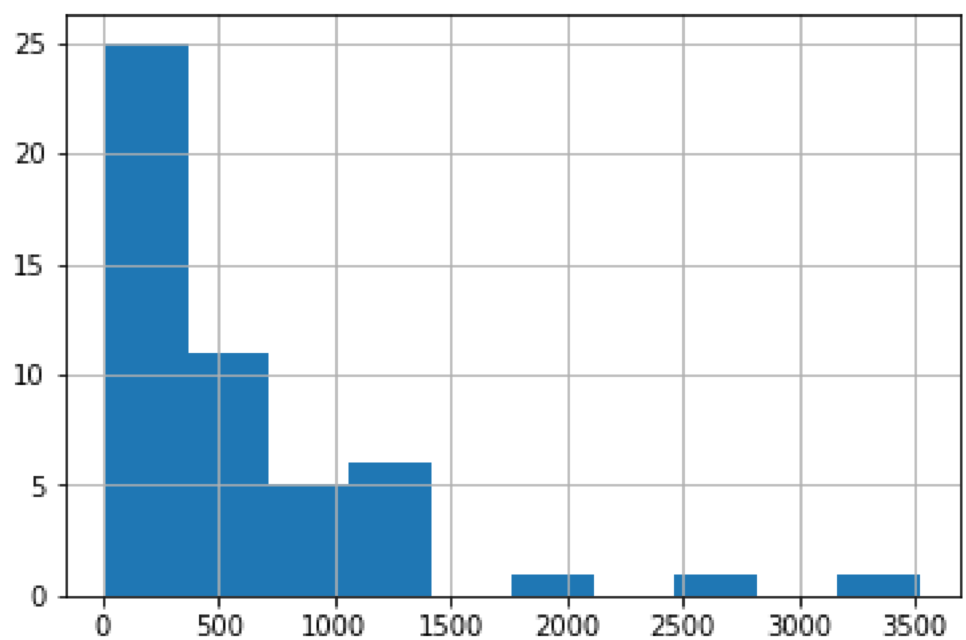
In [12]:
```
pyemu.os_utils.start_slaves(t_d,"pestpp-glm","freyberg_pp.pst",num_slaves=20,slave_ro
                            master_dir=m_d)
```

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
5      14.190950
24     39.816903
12     52.523092
32     56.304627
23     73.111480
39     86.050334
```

```
10     87.438308
49     96.953363
16    110.996486
15    115.277380
44    115.848527
29    137.807480
1     143.815281
17    143.834155
34    179.238577
11    197.914076
35    215.975898
37    217.419830
4     254.336227
6     275.840608
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:

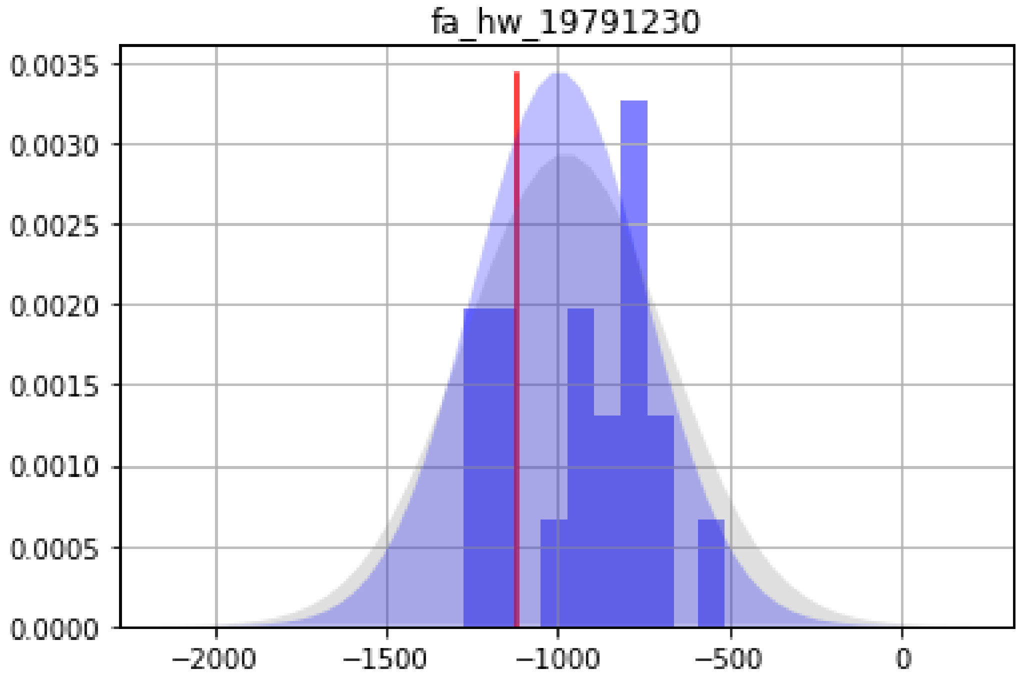
```
In [16]: f_df = pd.read_csv(os.path.join(m_d,"freyberg_pp.pred.usum.csv"),index_col=0)
         f_df.index = f_df.index.map(str.lower)
         f_df
```

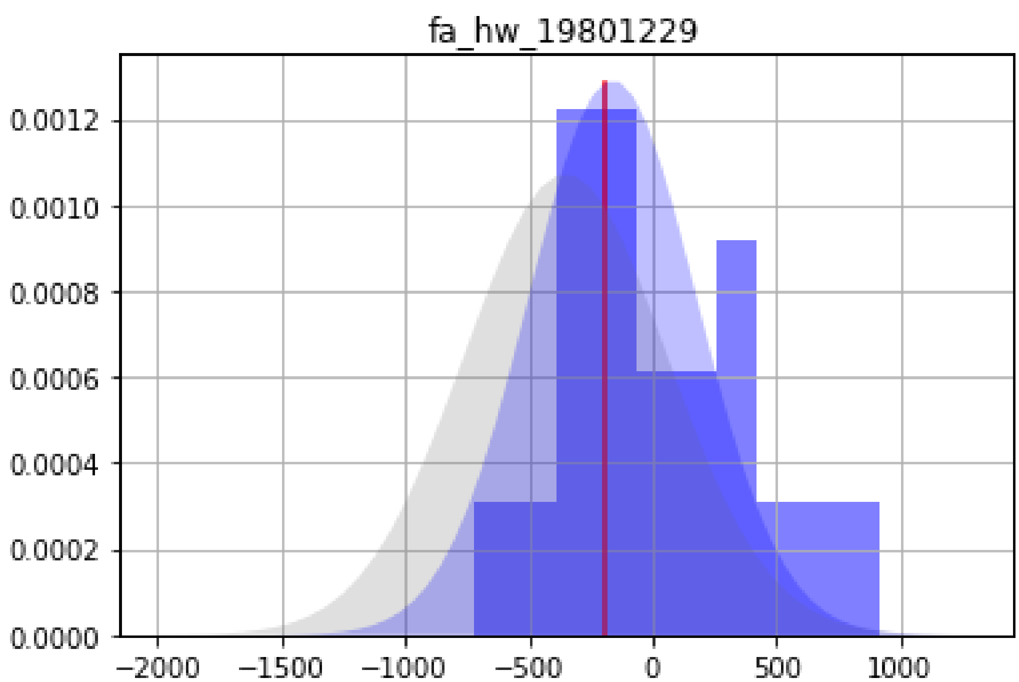
Out[16]:

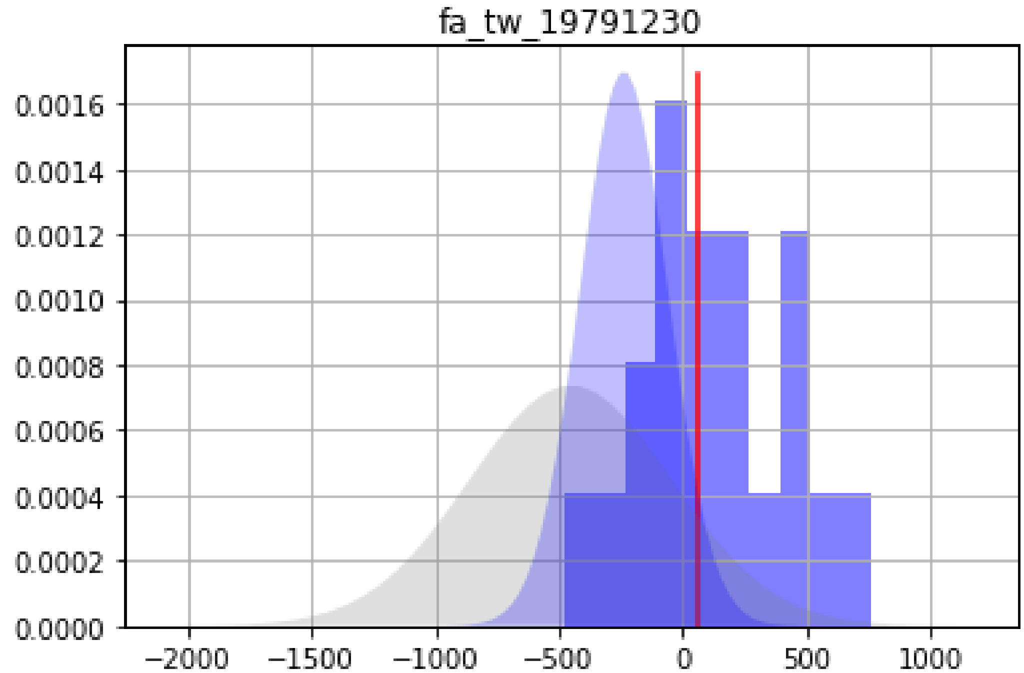
```
                     prior_mean  prior_stdev  prior_lower_bound  \
name
fa_hw_19791230        -977.2390    295.32800         -1567.8900
fa_hw_19801229        -351.2160    409.77000         -1170.7600
fa_tw_19791230        -453.0330    409.35100         -1271.7400
fa_tw_19801229         108.9600    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  -996.6270  251.312000
fa_hw_19801229                468.3240  -161.2820  340.513000
fa_tw_19791230                365.6690  -238.2400  177.440000
fa_tw_19801229               1122.4200   438.1610  270.099000
hds_00_013_002_000             47.5365    36.9962    0.311487
hds_00_013_002_001             46.4994    35.6765    0.703358
part_status                     2.0000     1.0000    0.000000
part_time                    2049.6700  4015.0000  439.930000

                     post_lower_bound  post_upper_bound
name
fa_hw_19791230             -1499.2500         -494.0040
fa_hw_19801229              -842.3070          519.7430
fa_tw_19791230              -593.1210          116.6410
fa_tw_19801229              -102.0380          978.3590
hds_00_013_002_000            36.3732           37.6192
hds_00_013_002_001            34.2698           37.0832
part_status                    1.0000            1.0000
part_time                   3135.1400         4894.8600
```

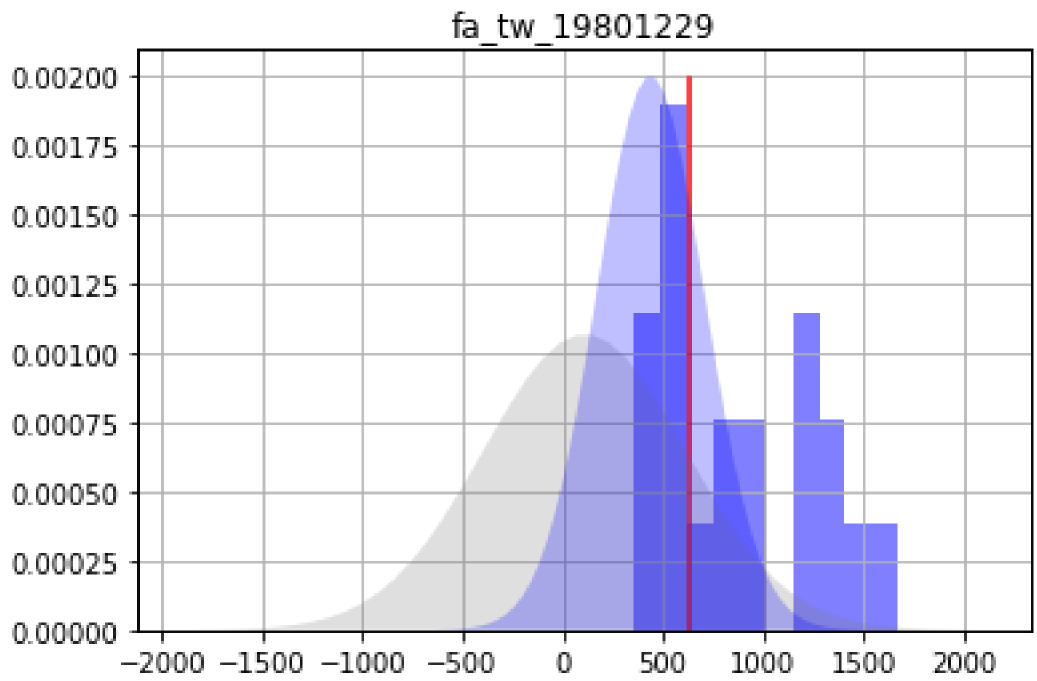
In [17]:

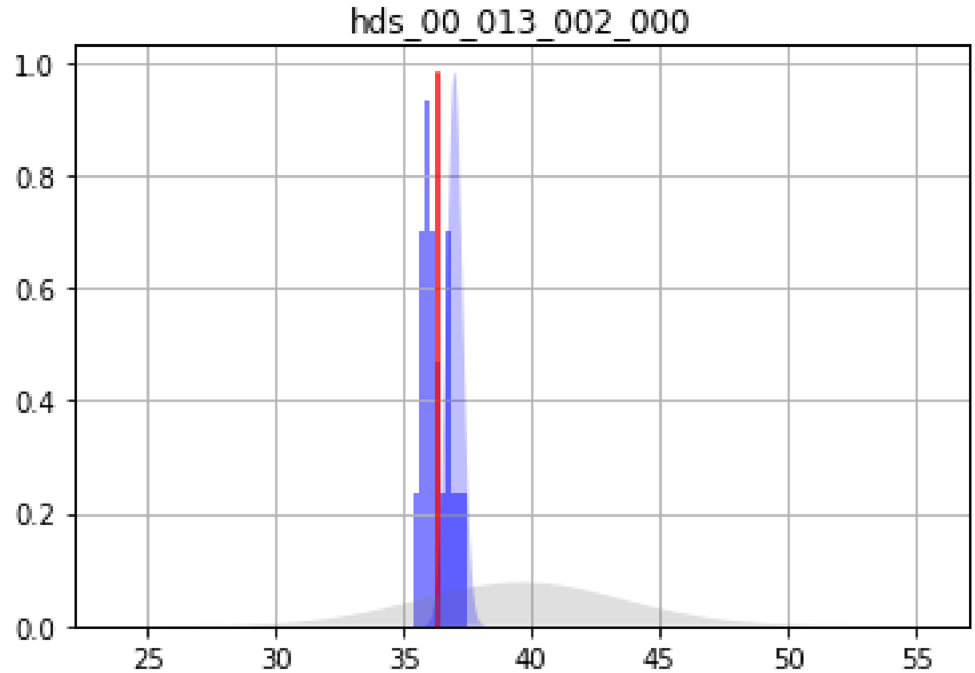
```
obs = pst.observation_data
fnames = pst.pestpp_options["forecasts"].split(",")
for forecast in fnames:
    ax = plt.subplot(111)
    oe_pt.loc[:,forecast].hist(ax=ax,color="b",alpha=0.5,normed=True)
    ax.plot([obs.loc[forecast,"obsval"],obs.loc[forecast,"obsval"]],ax.get_ylim(),"r"
    axt = plt.twinx()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

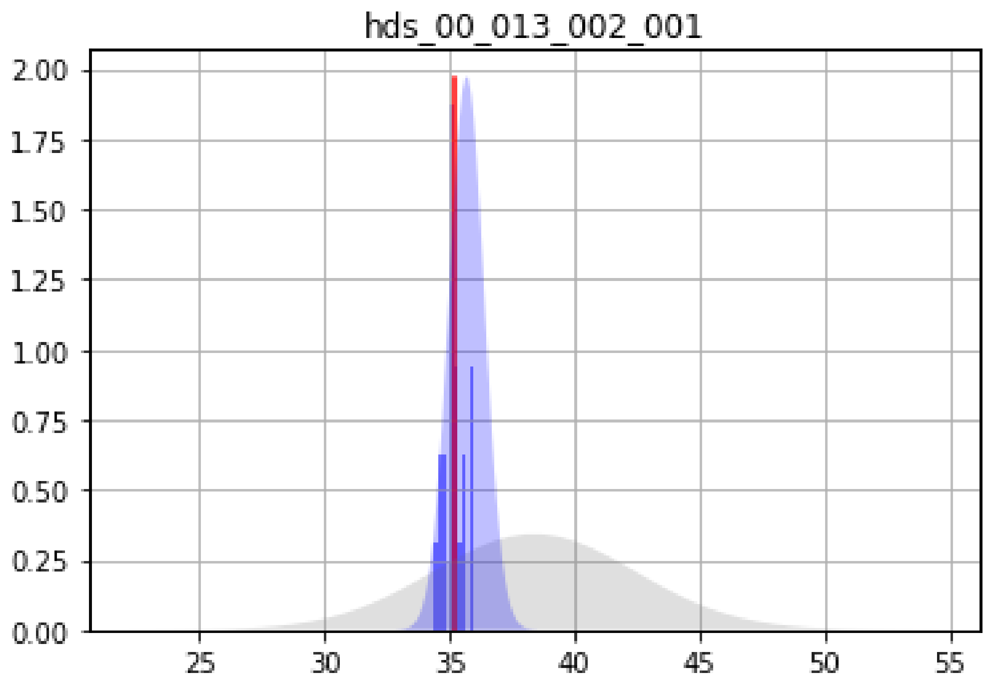

fa_hw_19791230
0.0035
0.0030
0.0025
0.0020
0.0015
0.0010
0.0005
0.0000
−2000
−1500
−1000
−500
0

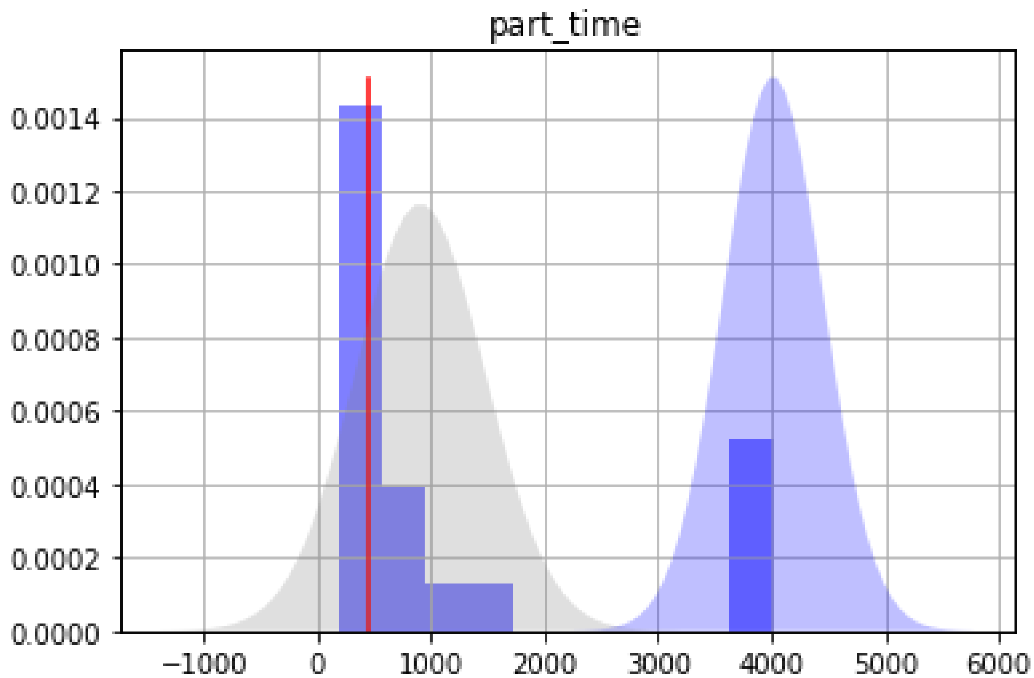

fa_hw_19801229
0.0012
0.0010
0.0008
0.0006
0.0004
0.0002
0.0000
−2000
−1500
−1000
−500
0
500
1000

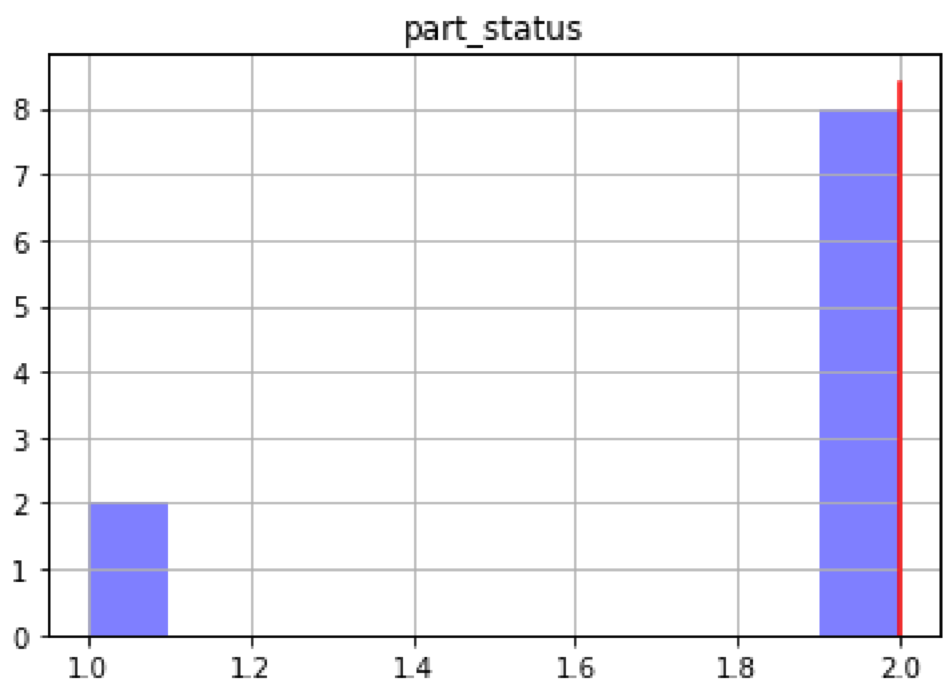

fa_tw_19791230
0.0016
0.0014
0.0012
0.0010
0.0008
0.0006
0.0004
0.0002
0.0000
−2000
−1500
−1000
−500
0
500
1000


fa_tw_19801229
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
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
2.00
1.75
1.50
1.25
1.00
0.75
0.50
0.25
0.00
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
−1000
0
1000
2000
3000
4000
5000
6000


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"))
```

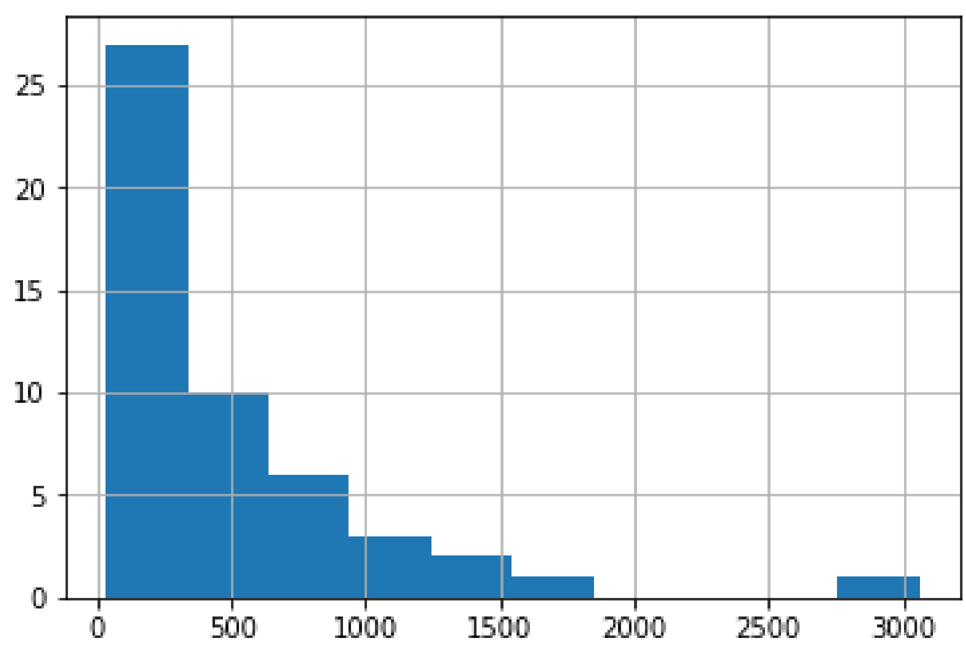
```
noptmax:3, npar_adj:527, nnz_obs:14
```

```
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
48     32.357636
39     44.490563
5      44.725659
44     54.782531
10     61.966469
1      62.102336
17     63.763626
11     74.117138
36    111.545765
15    122.623013
6     125.876614
38    128.385068
16    142.446552
49    145.750406
23    146.489583
45    149.032915
12    151.442470
33    163.005675
47    192.938712
27    201.362180
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:

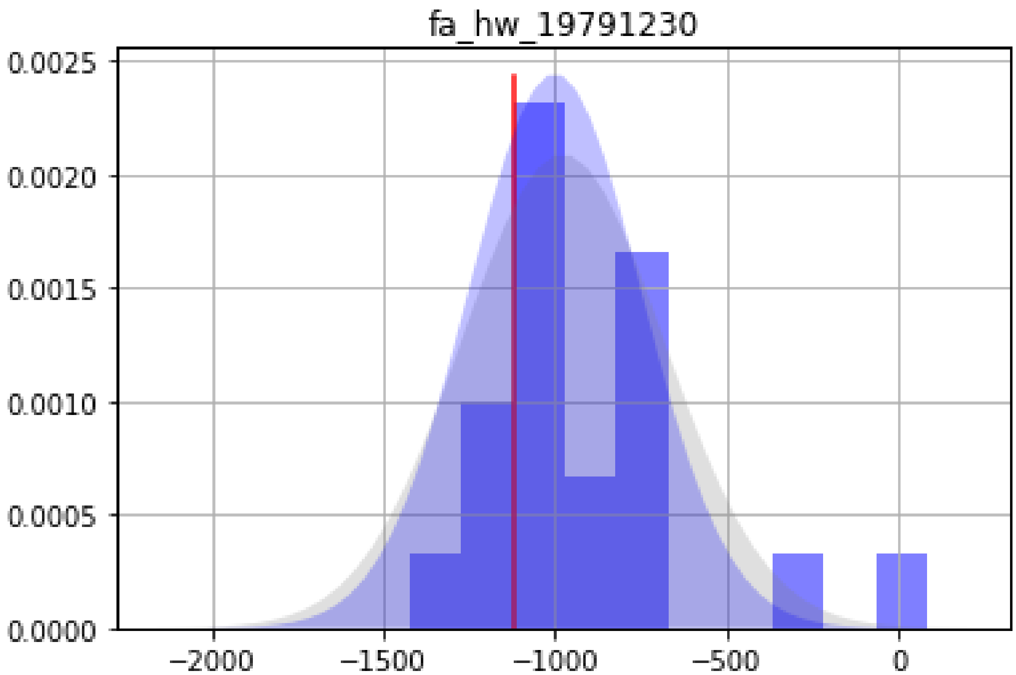
```
In [26]: oe_pt = oe.loc[oe.phi_vector.sort_values().index[:20],:]
```

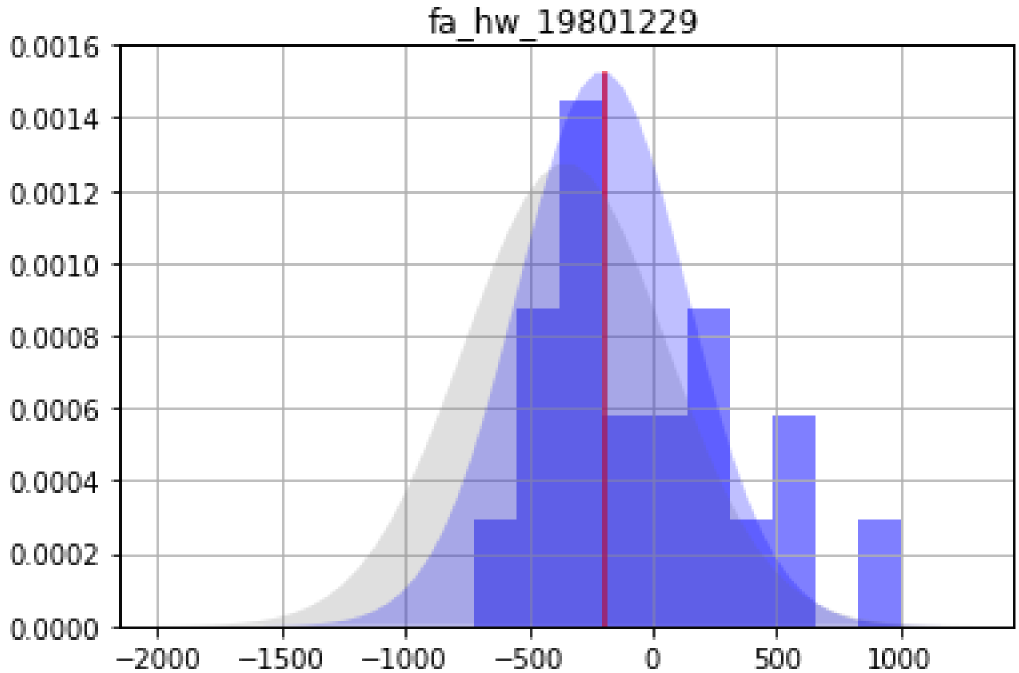
```
In [27]: f_df = pd.read_csv(os.path.join(m_d,"freyberg_pp.pred.usum.csv"),index_col=0)
         f_df.index = f_df.index.map(str.lower)
         f_df
```

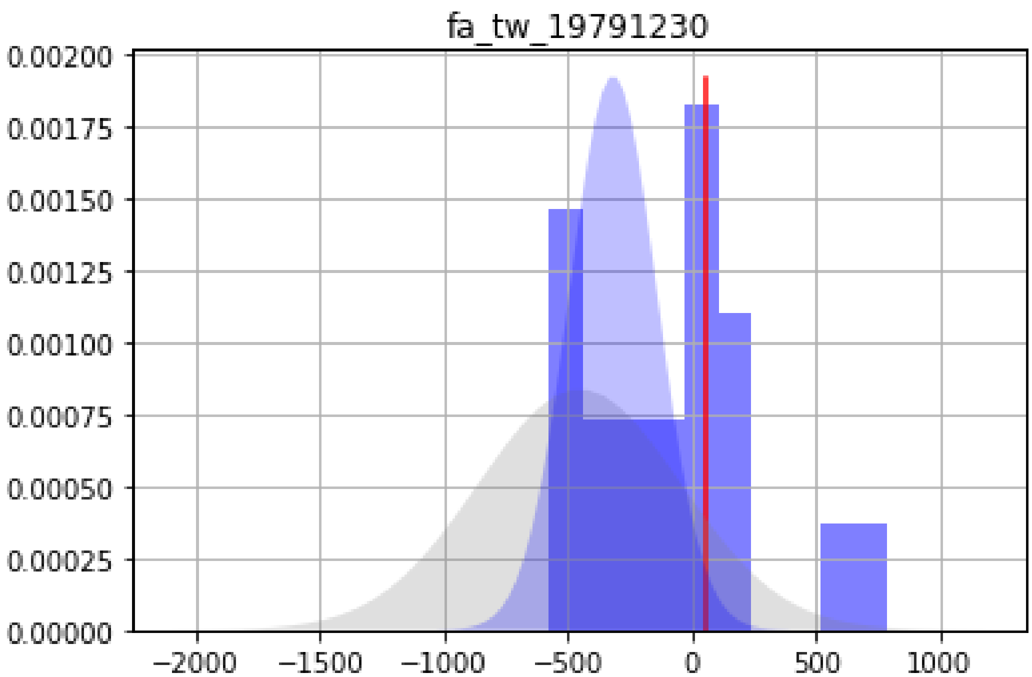
```
Out[27]:                      prior_mean  prior_stdev  prior_lower_bound  \
         name
         fa_hw_19791230        -977.2390    295.32800         -1567.8900
         fa_hw_19801229        -351.2160    409.77000         -1170.7600
         fa_tw_19791230        -453.0330    409.35100         -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    570.98600          -234.2690

                             prior_upper_bound  post_mean  post_stdev  \
         name
         fa_hw_19791230              -386.5840 -1000.4100  252.324000
         fa_hw_19801229               468.3240  -202.8870  342.087000
         fa_tw_19791230               365.6690  -317.6190  177.828000
         fa_tw_19801229              1122.4200   350.5420  270.291000
         hds_00_013_002_000            47.5365    37.3082    0.385044
         hds_00_013_002_001            46.4994    36.0158    0.738115
         part_status                    2.0000     2.0000    0.000000
         part_time                   2049.6700   989.9410  443.961000

                             post_lower_bound  post_upper_bound
         name
         fa_hw_19791230            -1505.0600         -495.7660
         fa_hw_19801229             -887.0620          481.2880
         fa_tw_19791230             -673.2750           38.0358
         fa_tw_19801229             -190.0410          891.1240
         hds_00_013_002_000           36.5381           38.0783
         hds_00_013_002_001           34.5396           37.4920
         part_status                   2.0000            2.0000
         part_time                   102.0190         1877.8600
```

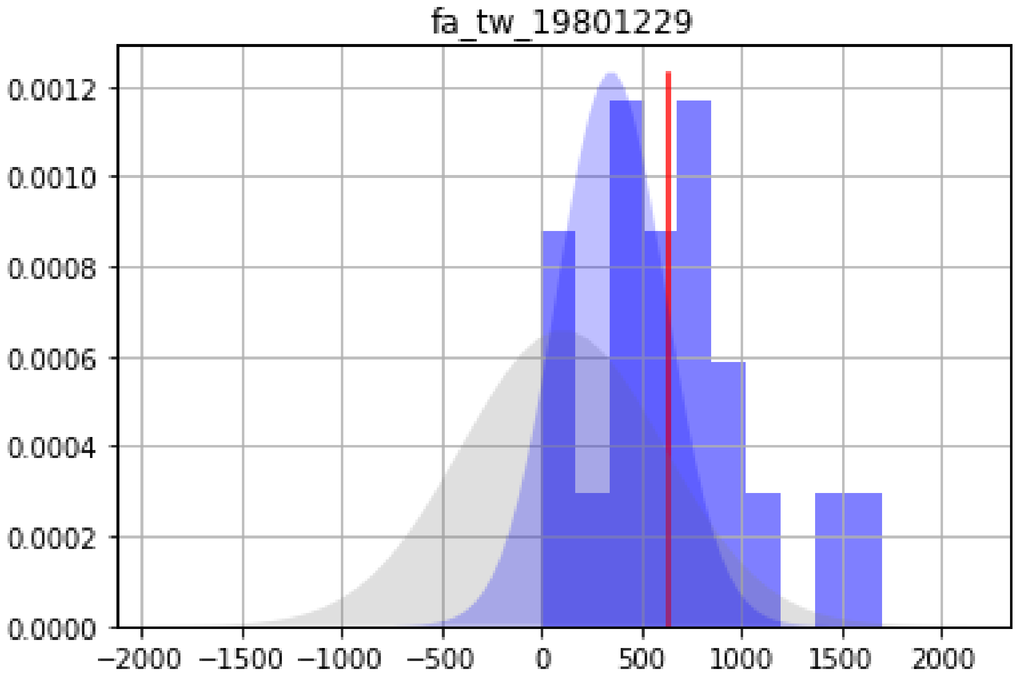
```
In [28]: obs = pst.observation_data
         fnames = pst.pestpp_options["forecasts"].split(",")
         for forecast in fnames:
             ax = plt.subplot(111)
             oe_pt.loc[:,forecast].hist(ax=ax,color="b",alpha=0.5,normed=True)
             ax.plot([obs.loc[forecast,"obsval"],obs.loc[forecast,"obsval"]],ax.get_ylim(),"r"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

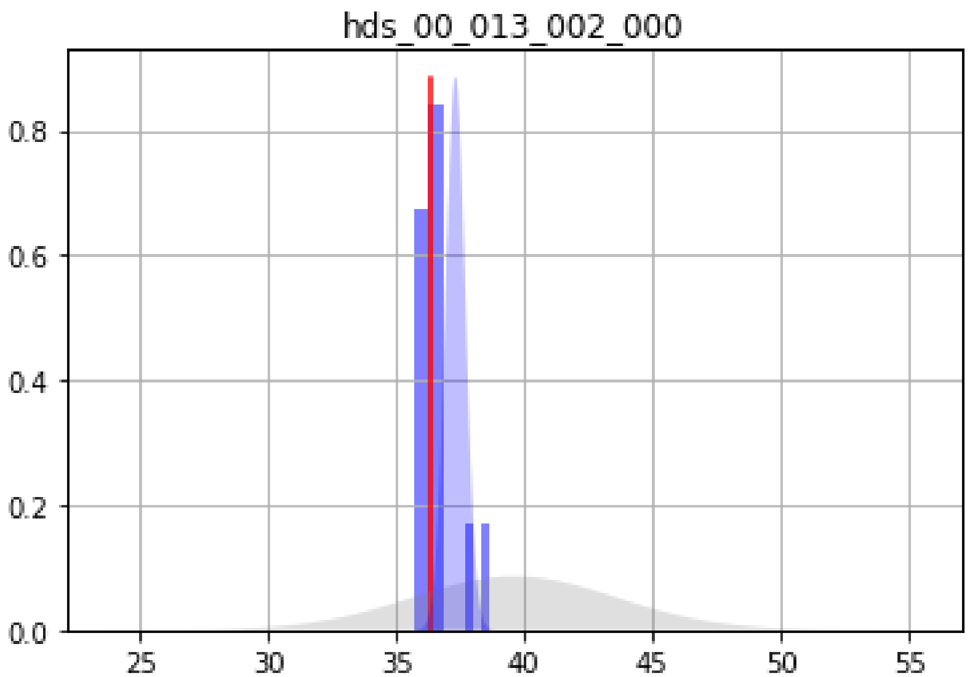
```
x,y = pyemu.plot_utils.gaussian_distribution(f_df.loc[forecast,"prior_mean"],f_df
axt.fill_between(x,0,y,facecolor="0.5",alpha=0.25)
x,y = pyemu.plot_utils.gaussian_distribution(f_df.loc[forecast,"post_mean"],f_df.l
axt.fill_between(x,0,y,facecolor="b",alpha=0.25)
axt.set_ylim(0,axt.get_ylim()[1])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

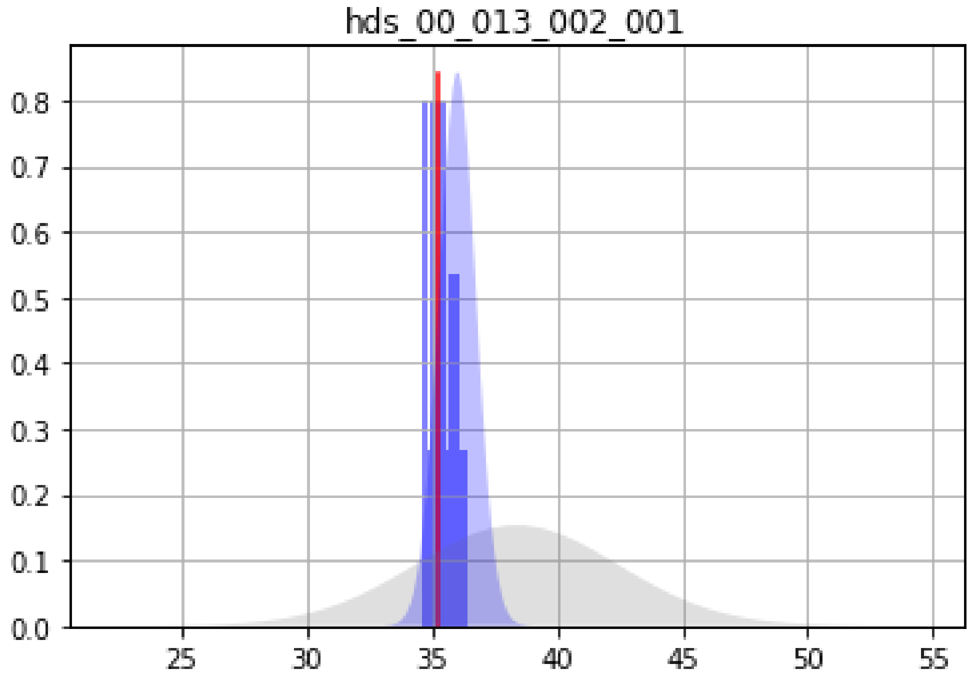


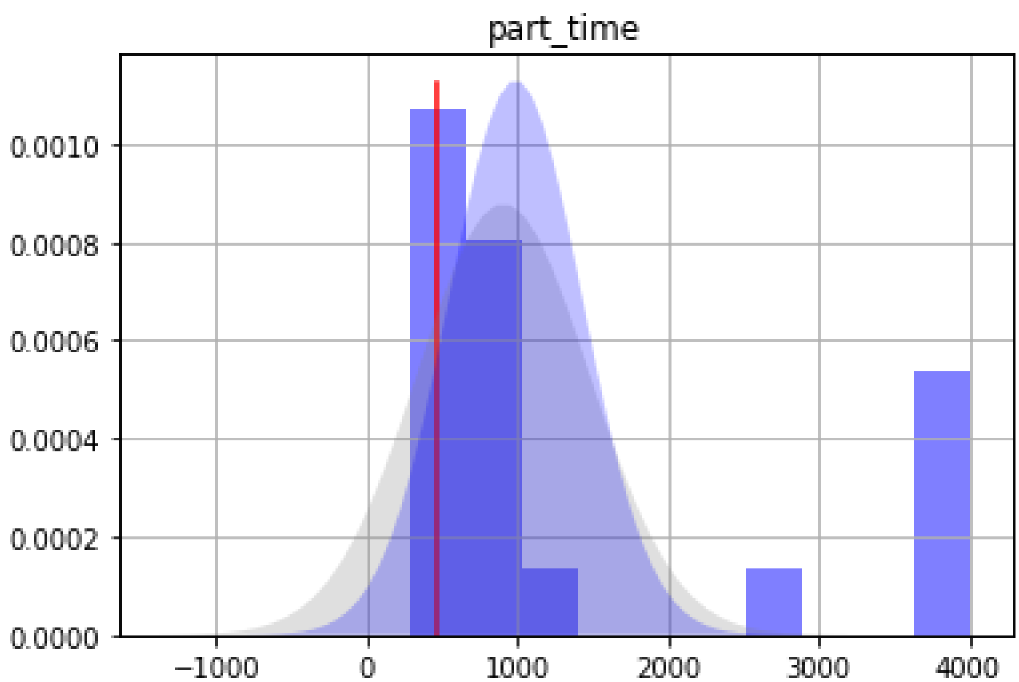

fa_hw_19801229
0.0016
0.0014
0.0012
0.0010
0.0008
0.0006
0.0004
0.0002
0.0000
−2000
−1500
−1000
−500
0
500
1000

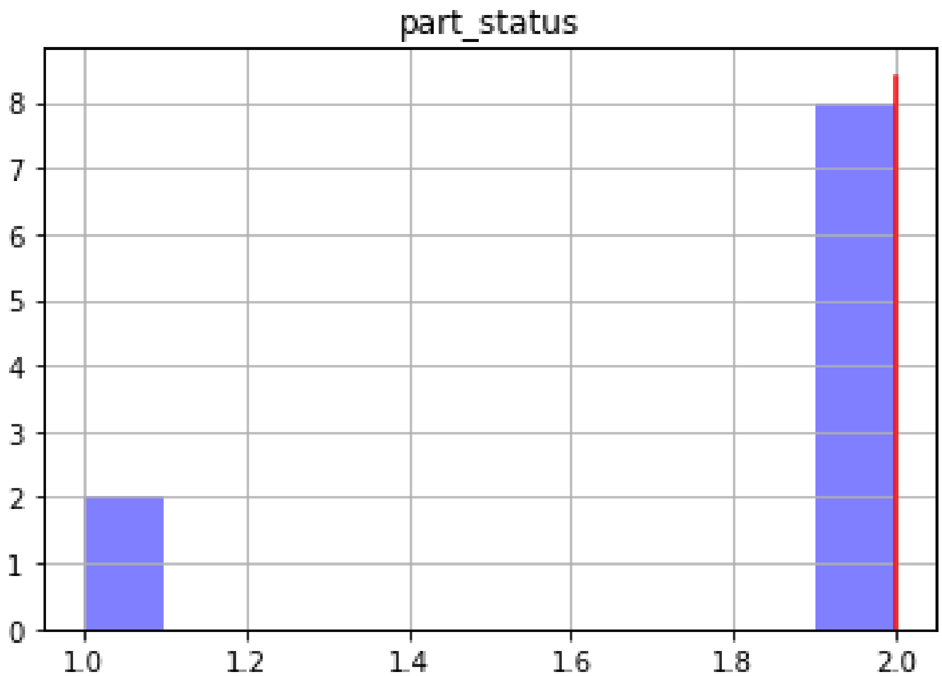

fa_tw_19791230
0.00200
0.00175
0.00150
0.00125
0.00100
0.00075
0.00050
0.00025
0.00000
−2000
−1500
−1000
−500
0
500
1000


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


hds_00_013_002_001
0.8
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
0.0010
0.0008
0.0006
0.0004
0.0002
0.0000
−1000
0
1000
2000
3000
4000


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