pestpp-glm

June 5, 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]: %matplotlib inline
        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
```

1.1 SUPER IMPORTANT: SET HOW MANY PARALLEL WORKERS TO USE

```
In [2]: num_workers = 20
```

```
In [3]: t_d = "template"
        m_d = "master_glm"
```

```
In [4]: pst = pyemu.Pst(os.path.join(t_d,"freyberg.pst"))
        pst.write_par_summary_table(filename="none")
```

```
Out[4]:                      type transform  count      initial value  \
        cn_strt8         cn_strt8       log      1                  0
        pp_prsity0     pp_prsity0       log     32                  0
        cn_prsity7     cn_prsity7       log      1                  0
        pp_strt2         pp_strt2       log     32                  0
        pp_strt0         pp_strt0       log     32                  0
        cn_hk7              cn_hk7      log      1                  0
        pp_vka1           pp_vka1       log     32                  0
```

gr_vka5	gr_vka5	log	705	0
pp_hk2	pp_hk2	log	32	0
cn_prsity6	cn_prsity6	log	1	0
pp_rech1	pp_rech1	log	32	0
pp_prsity2	pp_prsity2	log	32	0
pp_sy2	pp_sy2	log	32	0
gr_rech2	gr_rech2	log	705	0
gr_rech3	gr_rech3	log	705	0
pp_sy1	pp_sy1	log	32	0
cn_rech5	cn_rech5	log	1	-0.39794
cn_strt7	cn_strt7	log	1	0
gr_strt4	gr_strt4	log	705	0
welflux_k02	welflux_k02	log	6	0
pp_sy0	pp_sy0	log	32	0
gr_strt3	gr_strt3	log	705	0
welflux	welflux	log	2	0 to 0.176091
cn_vka6	cn_vka6	log	1	0
cn_strt6	cn_strt6	log	1	0
gr_ss5	gr_ss5	log	705	0
cn_ss7	cn_ss7	log	1	0
gr_hk5	gr_hk5	log	705	0
cn_ss8	cn_ss8	log	1	0
gr_vka3	gr_vka3	log	705	0
...	...	...	...	...
pp_hk1	pp_hk1	log	32	0
pp_hk0	pp_hk0	log	32	0
gr_prsity5	gr_prsity5	log	705	0
pp_ss1	pp_ss1	log	32	0
cn_sy8	cn_sy8	log	1	0
gr_ss4	gr_ss4	log	705	0
gr_vka4	gr_vka4	log	705	0
pp_strt1	pp_strt1	log	32	0
cn_vka7	cn_vka7	log	1	0
pp_ss2	pp_ss2	log	32	0
drncond_k00	drncond_k00	log	10	0
gr_sy4	gr_sy4	log	705	0
cn_vka8	cn_vka8	log	1	0
gr_prsity4	gr_prsity4	log	705	0
cn_hk6	cn_hk6	log	1	0
flow	flow	log	1	0
cn_rech4	cn_rech4	log	1	0
pp_rech0	pp_rech0	log	32	0
gr_sy5	gr_sy5	log	705	0
cn_prsity8	cn_prsity8	log	1	0
pp_vka0	pp_vka0	log	32	0
pp_vka2	pp_vka2	log	32	0
gr_hk3	gr_hk3	log	705	0
gr_strt5	gr_strt5	log	705	0

gr_hk4	gr_hk4	log	705	0
cn_sy6	cn_sy6	log	1	0
pp_ss0	pp_ss0	log	32	0
cn_sy7	cn_sy7	log	1	0
gr_prsity3	gr_prsity3	log	705	0
cn_hk8	cn_hk8	log	1	0

	upper bound	lower bound	standard deviation
cn_strt8	0.0211893	-0.0222764	0.0108664
pp_prsity0	0.176091	-0.30103	0.11928
cn_prsity7	0.176091	-0.30103	0.11928
pp_strt2	0.0211893	-0.0222764	0.0108664
pp_strt0	0.0211893	-0.0222764	0.0108664
cn_hk7	1	-1	0.5
pp_vka1	1	-1	0.5
gr_vka5	1	-1	0.5
pp_hk2	1	-1	0.5
cn_prsity6	0.176091	-0.30103	0.11928
pp_rech1	0.0413927	-0.0457575	0.0217875
pp_prsity2	0.176091	-0.30103	0.11928
pp_sy2	0.243038	-0.60206	0.211275
gr_rech2	0.0413927	-0.0457575	0.0217875
gr_rech3	0.0413927	-0.0457575	0.0217875
pp_sy1	0.243038	-0.60206	0.211275
cn_rech5	-0.09691	-1	0.225772
cn_strt7	0.0211893	-0.0222764	0.0108664
gr_strt4	0.0211893	-0.0222764	0.0108664
welflux_k02	1	-1	0.5
pp_sy0	0.243038	-0.60206	0.211275
gr_strt3	0.0211893	-0.0222764	0.0108664
welflux	0.176091 to 0.30103	-0.30103 to 0	0.0752575 to 0.11928
cn_vka6	1	-1	0.5
cn_strt6	0.0211893	-0.0222764	0.0108664
gr_ss5	1	-1	0.5
cn_ss7	1	-1	0.5
gr_hk5	1	-1	0.5
cn_ss8	1	-1	0.5
gr_vka3	1	-1	0.5
...	...	...	...
pp_hk1	1	-1	0.5
pp_hk0	1	-1	0.5
gr_prsity5	0.176091	-0.30103	0.11928
pp_ss1	1	-1	0.5
cn_sy8	0.243038	-0.60206	0.211275
gr_ss4	1	-1	0.5
gr_vka4	1	-1	0.5
pp_strt1	0.0211893	-0.0222764	0.0108664
cn_vka7	1	-1	0.5

```
pp_ss2                  1          -1          0.5
drncond_k00             1          -1          0.5
gr_sy4           0.243038    -0.60206     0.211275
cn_vka8                 1          -1          0.5
gr_prsity4       0.176091    -0.30103      0.11928
cn_hk6                  1          -1          0.5
flow              0.09691   -0.124939    0.0554622
cn_rech4        0.0791812    -0.09691    0.0440228
pp_rech0        0.0413927  -0.0457575    0.0217875
gr_sy5           0.243038    -0.60206     0.211275
cn_prsity8       0.176091    -0.30103      0.11928
pp_vka0                 1          -1          0.5
pp_vka2                 1          -1          0.5
gr_hk3                  1          -1          0.5
gr_strt5        0.0211893  -0.0222764    0.0108664
gr_hk4                  1          -1          0.5
cn_sy6           0.243038    -0.60206     0.211275
pp_ss0                  1          -1          0.5
cn_sy7           0.243038    -0.60206     0.211275
gr_prsity3       0.176091    -0.30103      0.11928
cn_hk8                  1          -1          0.5

[65 rows x 7 columns]
```

1.1.1 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 [5]: par = pst.parameter_data
```

```
In [6]: # 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[6]: 719
```

```
In [7]: # 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[7]: 719
```

```
In [8]: par.loc[par.pargp.apply(lambda x: "pp" in x),"pargp"].unique()
```

```
Out[8]: 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 [9]: #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[9]: 719
```

```
In [10]: adj_par = par.loc[par.partrans=="log",:]
         adj_par.pargp.value_counts().sort_values()
```

```
Out[10]: cn_hk8           1
         cn_hk6           1
         cn_prsity7       1
         cn_prsity8       1
         cn_hk7           1
         cn_rech4         1
         flow             1
         cn_prsity6       1
         cn_vka8          1
         cn_rech5         1
         cn_vka7          1
         cn_ss8           1
         cn_sy6           1
         cn_sy7           1
         cn_vka6          1
         cn_strt6         1
         cn_ss7           1
         cn_strt7         1
         cn_strt8         1
         cn_ss6           1
         cn_sy8           1
         welflux          2
         welflux_k02      6
         drncond_k00     10
         pp_ss2          32
         pp_ss0          32
         pp_hk0          32
         pp_rech0        32
         pp_strt2        32
         pp_strt0        32
         pp_vka1         32
```

```
pp_hk2         32
pp_rech1       32
pp_prsity2     32
pp_sy2         32
pp_sy0         32
pp_prsity1     32
pp_hk1         32
pp_prsity0     32
pp_ss1         32
pp_vka2        32
pp_strt1       32
pp_vka0        32
pp_sy1         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 [11]: 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[11]: 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 [12]: 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"))
```

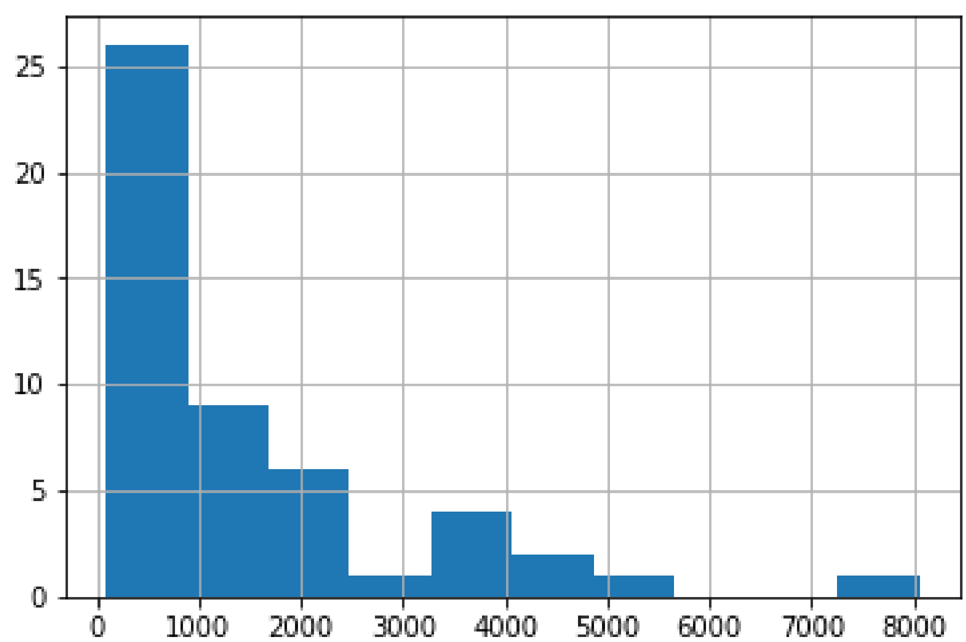
```
noptmax:3, npar_adj:527, nnz_obs:14
```

```
In [13]: pyemu.os_utils.start_slaves(t_d,"pestpp-glm","freyberg_pp.pst",num_slaves=num_workers
                                     master_dir=m_d)
```

```
In [14]: 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 [15]: ax = oe.phi_vector.hist()#bins=np.linspace(0,100,20))
         oe.phi_vector.sort_values().iloc[:20]
```

Out[15]:
```
real_name
16     93.563008
25    170.672590
11    215.054772
33    229.920615
6     246.861326
24    251.063969
45    272.209134
23    279.243029
37    322.455007
26    332.400050
21    343.341730
48    354.597653
34    401.095146
46    408.511642
7     420.700508
39    441.698089
42    442.051026
12    489.628147
3     489.754867
10    545.568931
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 [16]: oe_pt = oe.loc[oe.phi_vector.sort_values().index[:20],:] #just take the 20 lowest phi
```

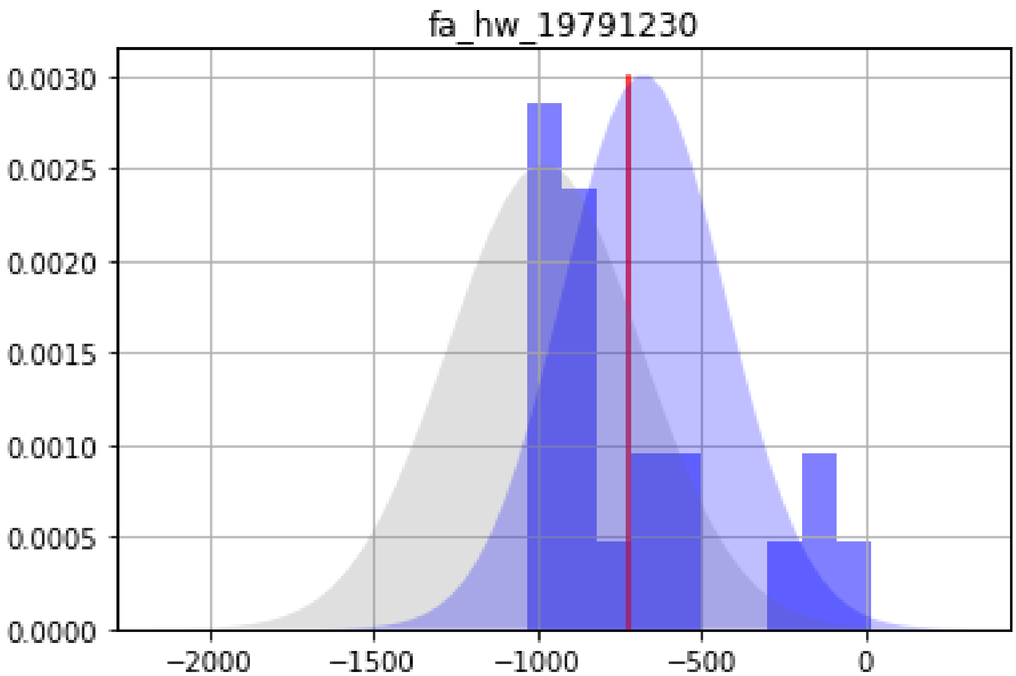
We can also load and plot the FOSM forecast results along side of the ensemble results:

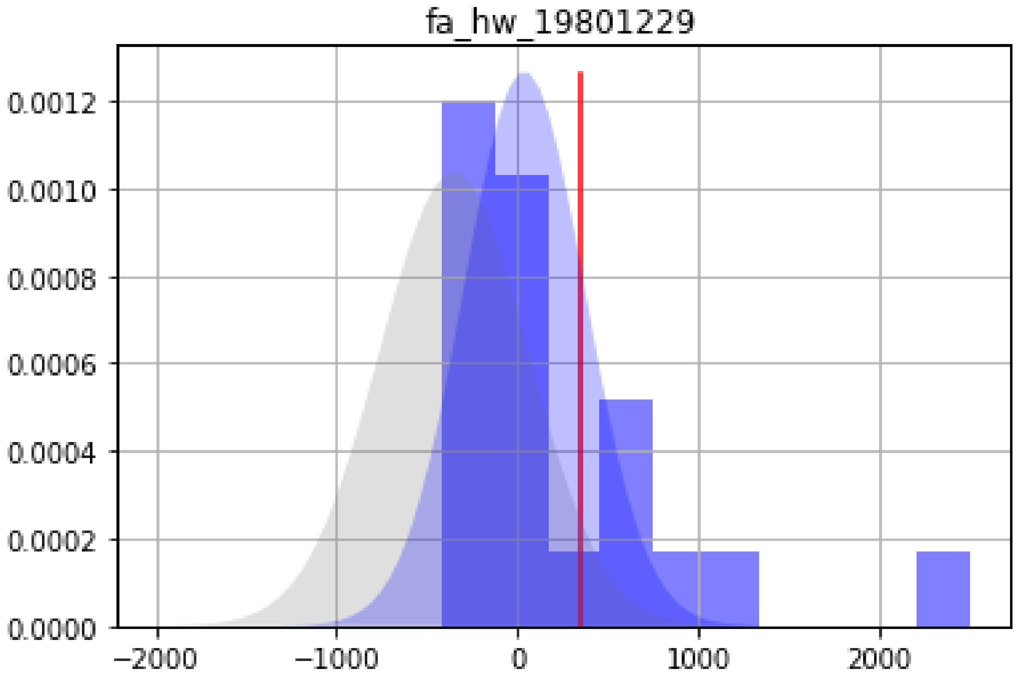
```
In [17]: f_df = pd.read_csv(os.path.join(m_d,"freyberg_pp.pred.usum.csv"),index_col=0)
         f_df.index = f_df.index.map(str.lower)
         f_df
```

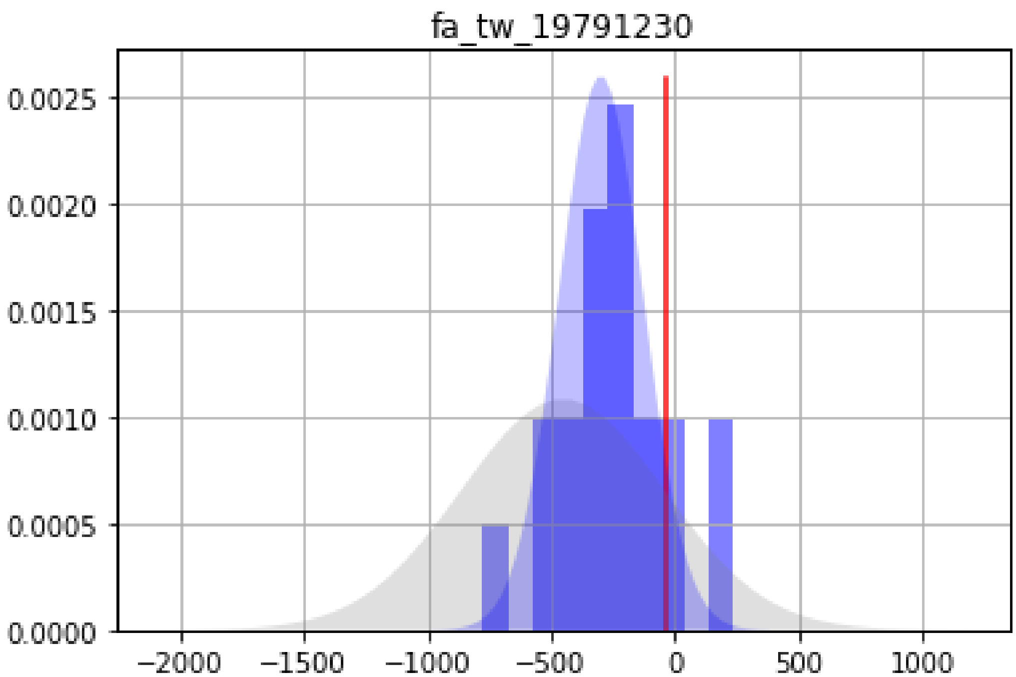
```
Out[17]:                      prior_mean  prior_stdev  prior_lower_bound  \
         name
         fa_hw_19791230        -977.2390    295.32800         -1567.8900
         fa_hw_19801229        -351.2160    409.77000         -1170.7600
         fa_tw_19791230        -453.0330    409.35100         -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  -675.0430  247.837000
         fa_hw_19801229                468.3240    37.6125  335.549000
         fa_tw_19791230                365.6690  -299.4690  170.577000
         fa_tw_19801229               1122.4200   333.7460  263.672000
         hds_00_013_002_000             47.5365    37.6359    0.273990
         hds_00_013_002_001             46.4994    36.4927    0.687833
         part_status                     2.0000     2.0000    0.000000
         part_time                    2049.6700   703.9470  436.945000

                             post_lower_bound  post_upper_bound
         name
         fa_hw_19791230             -1170.7200         -179.3700
         fa_hw_19801229              -633.4850          708.7100
         fa_tw_19791230              -640.6230           41.6858
         fa_tw_19801229              -193.5970          861.0890
         hds_00_013_002_000            37.0879           38.1838
         hds_00_013_002_001            35.1171           37.8684
         part_status                    2.0000            2.0000
         part_time                   -169.9420         1577.8400
```

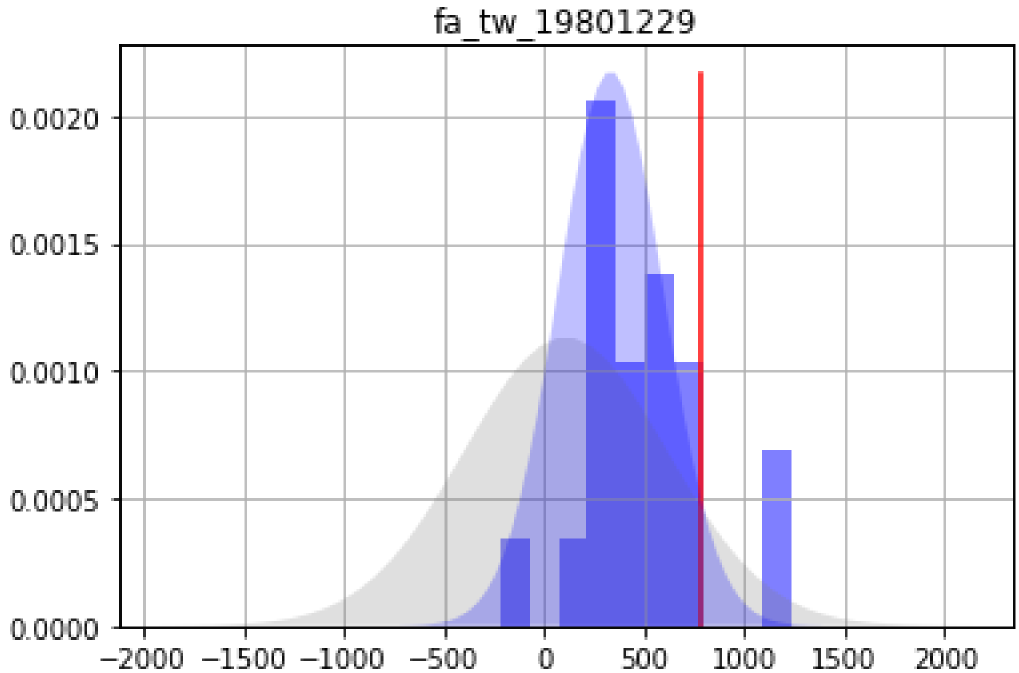
```
In [18]: obs = pst.observation_data
         fnames = pst.pestpp_options["forecasts"].split(",")
         for forecast in fnames:
             ax = plt.subplot(111)
             oe_pt.loc[:,forecast].hist(ax=ax,color="b",alpha=0.5,normed=True)
             ax.plot([obs.loc[forecast,"obsval"],obs.loc[forecast,"obsval"]],ax.get_ylim(),"r"
             axt = plt.twinx()
             x,y = pyemu.plot_utils.gaussian_distribution(f_df.loc[forecast,"prior_mean"],f_df
```

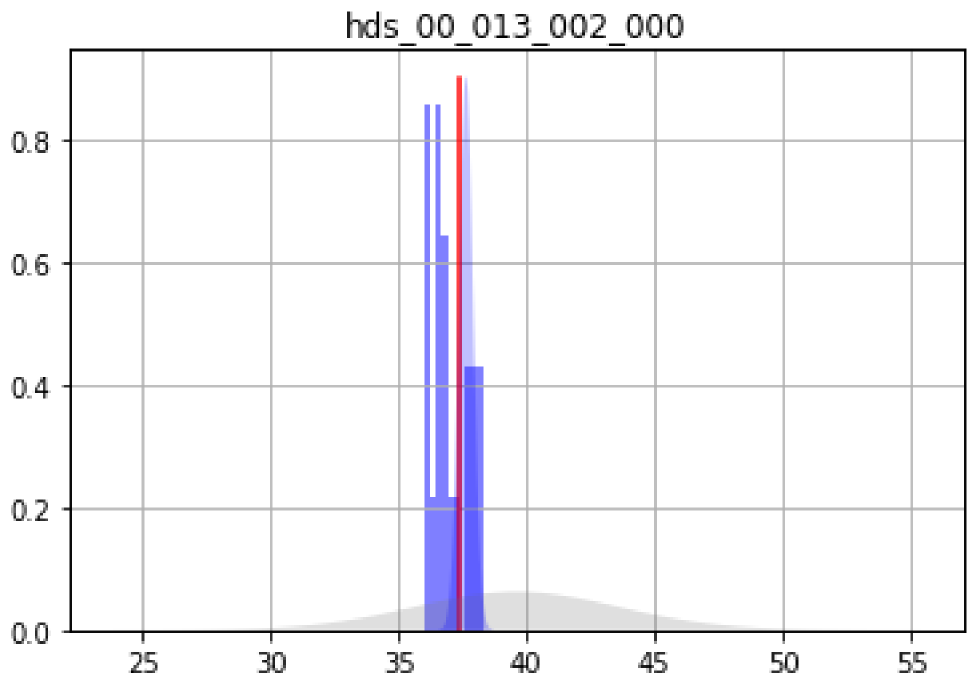
```
axt.fill_between(x,0,y,facecolor="0.5",alpha=0.25)
x,y = pyemu.plot_utils.gaussian_distribution(f_df.loc[forecast,"post_mean"],f_df.l
axt.fill_between(x,0,y,facecolor="b",alpha=0.25)
axt.set_ylim(0,axt.get_ylim()[1])
axt.set_yticks([])
ax.set_title(forecast)
plt.show()
```

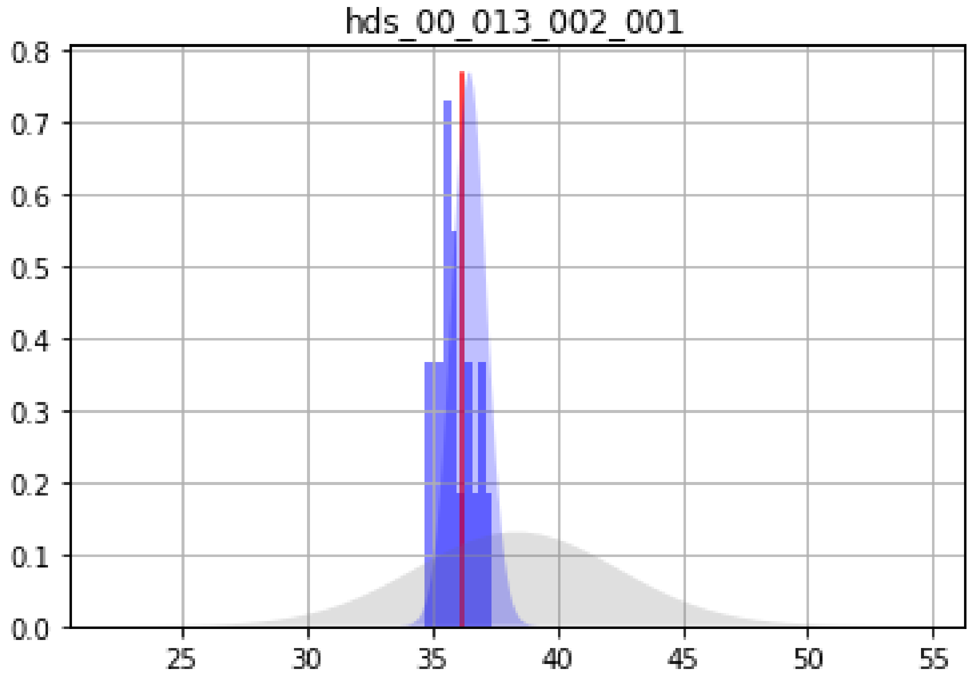


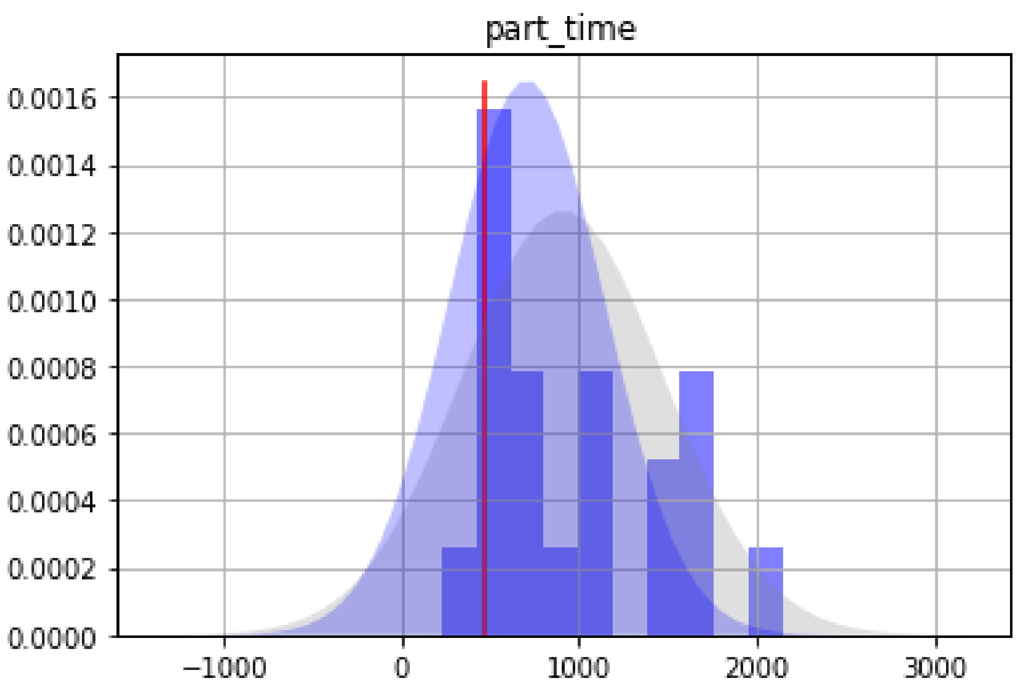

fa_hw_19801229
0.0012
0.0010
0.0008
0.0006
0.0004
0.0002
0.0000
−2000
−1000
0
1000
2000

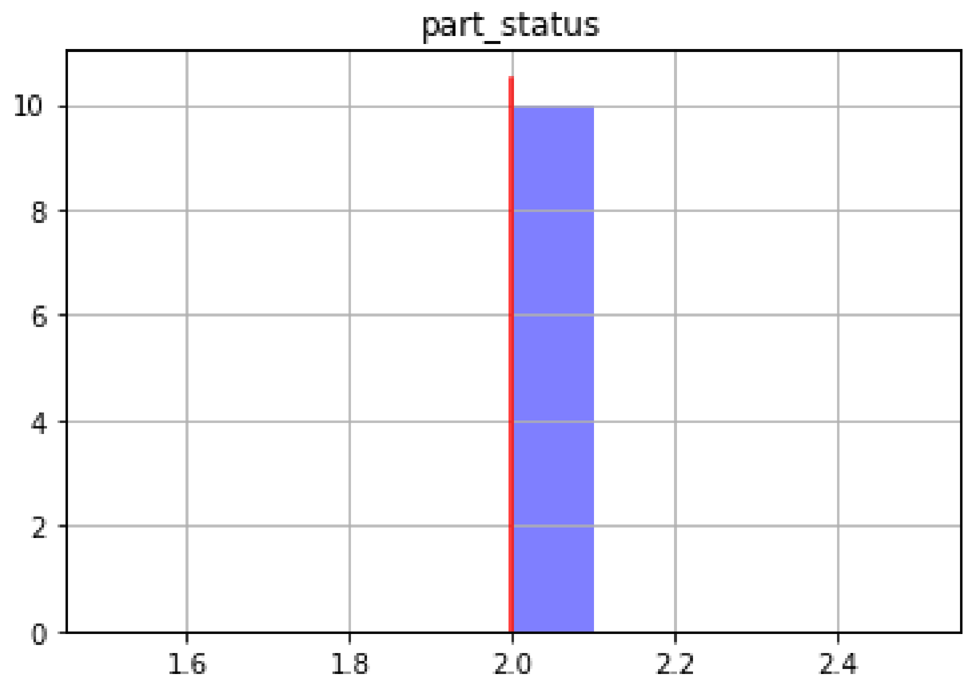

fa_tw_19791230
0.0025
0.0020
0.0015
0.0010
0.0005
0.0000
−2000
−1500
−1000
−500
0
500
1000


fa_tw_19801229
0.0020
0.0015
0.0010
0.0005
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
0.0016
0.0014
0.0012
0.0010
0.0008
0.0006
0.0004
0.0002
0.0000
−1000
0
1000
2000
3000



1.1.2 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 [19]: cov = pyemu.Cov.from_binary(os.path.join(t_d,"prior_cov.jcb"))
```

```
new binary format detected...
```

```
In [20]: pyemu.helpers.first_order_pearson_tikhonov(pst,cov)
```

```
getting CC matrix
processing
```

```
In [21]: pst.prior_information.head()
```

```
Out[21]:                                                      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 [22]:
```
shutil.copy2(os.path.join(m_d,"freyberg_pp.jcb"),os.path.join(t_d,"restart_pp.jcb"))
```

Out[22]:
```
'template/restart_pp.jcb'
```

In [23]:
```
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
```

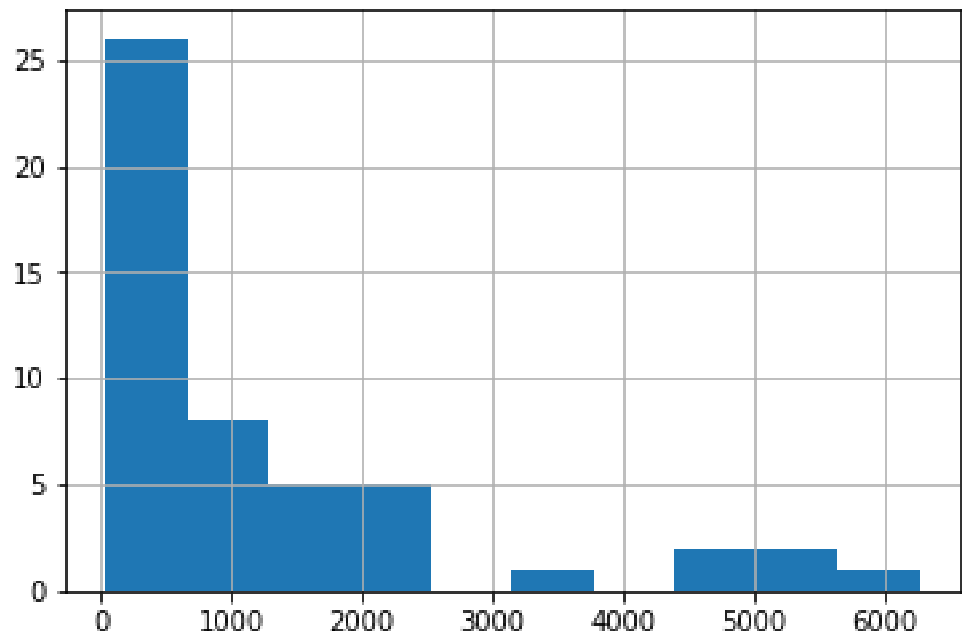
In [24]:
```
pyemu.os_utils.start_slaves(t_d,"pestpp-glm","freyberg_pp.pst",num_slaves=num_workers
                            master_dir=m_d)
```

In [25]:
```
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 [26]:
```
ax = oe.phi_vector.hist()#bins=np.linspace(0,100,20))
oe.phi_vector.sort_values().iloc[:20]
```

Out[26]:
```
real_name
46     41.263489
16     63.951582
35    121.513255
7     137.446945
11    208.807130
45    210.737423
12    261.316576
9     281.400104
47    321.419440
19    330.908864
24    331.863379
25    333.766324
39    352.884354
30    361.820742
26    383.330645
21    390.853366
15    408.456242
44    413.387639
```

```
1     498.360492
33    514.880477
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 [27]: oe_pt = oe.loc[oe.phi_vector.sort_values().index[:20],:]
```

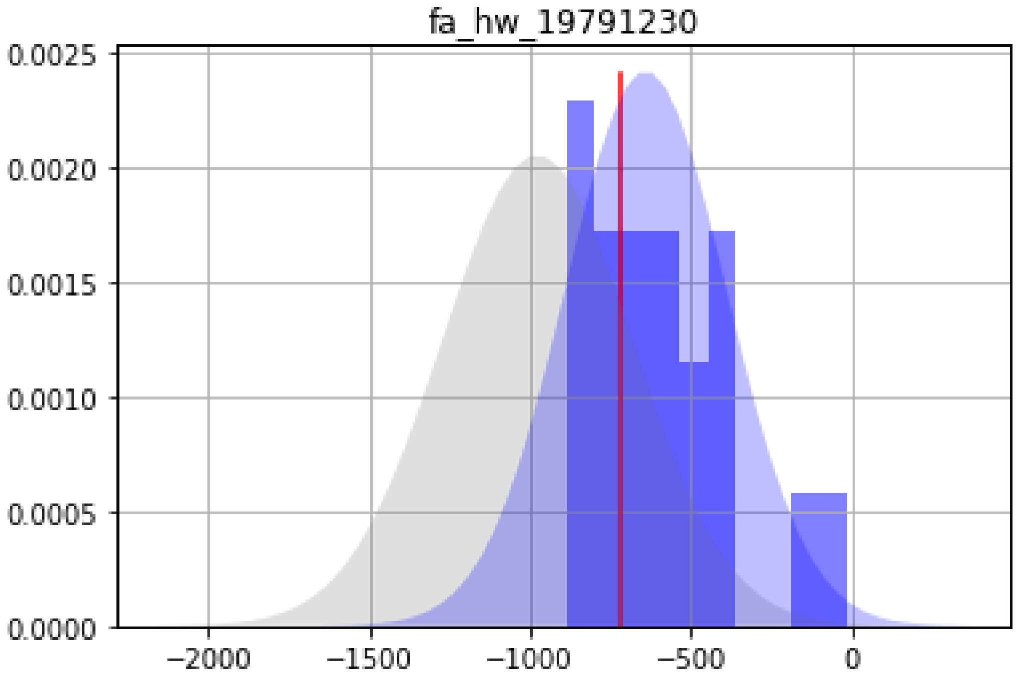
```
In [28]: f_df = pd.read_csv(os.path.join(m_d,"freyberg_pp.pred.usum.csv"),index_col=0)
         f_df.index = f_df.index.map(str.lower)
         f_df
```

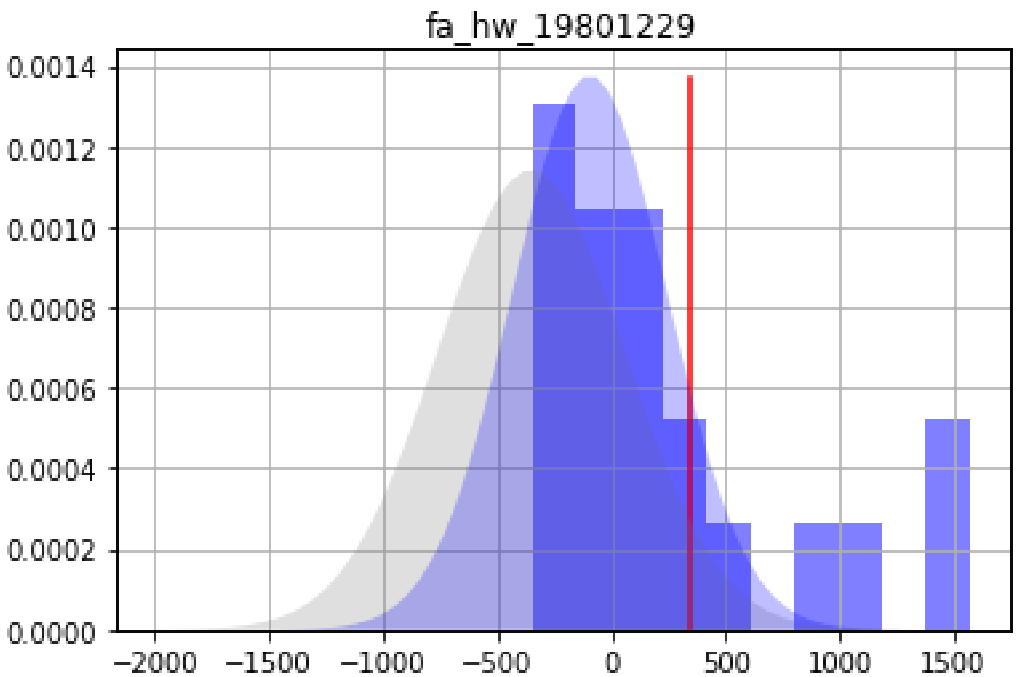
```
Out[28]:                      prior_mean  prior_stdev  prior_lower_bound  \
         name
         fa_hw_19791230        -977.2390    295.32800         -1567.8900
         fa_hw_19801229        -351.2160    409.77000         -1170.7600
         fa_tw_19791230        -453.0330    409.35100         -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  -640.3370  250.802000
```

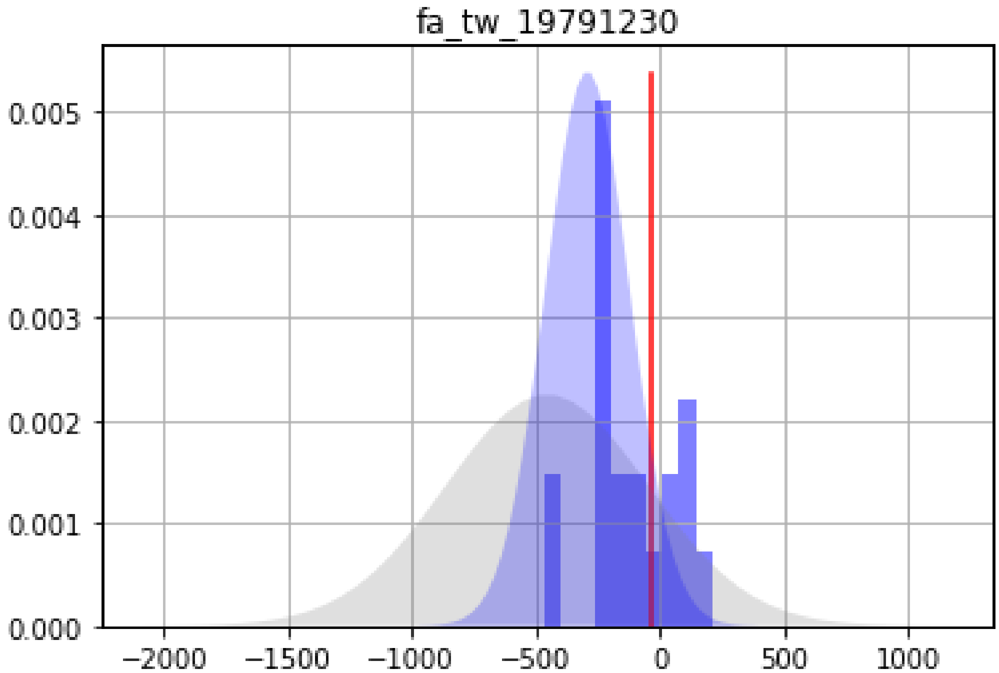
```
fa_hw_19801229              468.3240   -94.8227  339.971000
fa_tw_19791230              365.6690  -290.4730  170.616000
fa_tw_19801229             1122.4200   184.3570  263.999000
hds_00_013_002_000           47.5365    37.7893    0.274188
hds_00_013_002_001           46.4994    36.9350    0.687976
part_status                   2.0000     2.0000    0.000000
part_time                  2049.6700   966.2250  437.215000

                    post_lower_bound  post_upper_bound
name
fa_hw_19791230            -1141.9400         -138.7340
fa_hw_19801229             -774.7640          585.1190
fa_tw_19791230             -631.7040           50.7581
fa_tw_19801229             -343.6410          712.3540
hds_00_013_002_000           37.2409           38.3377
hds_00_013_002_001           35.5591           38.3110
part_status                   2.0000            2.0000
part_time                    91.7946         1840.6600
```

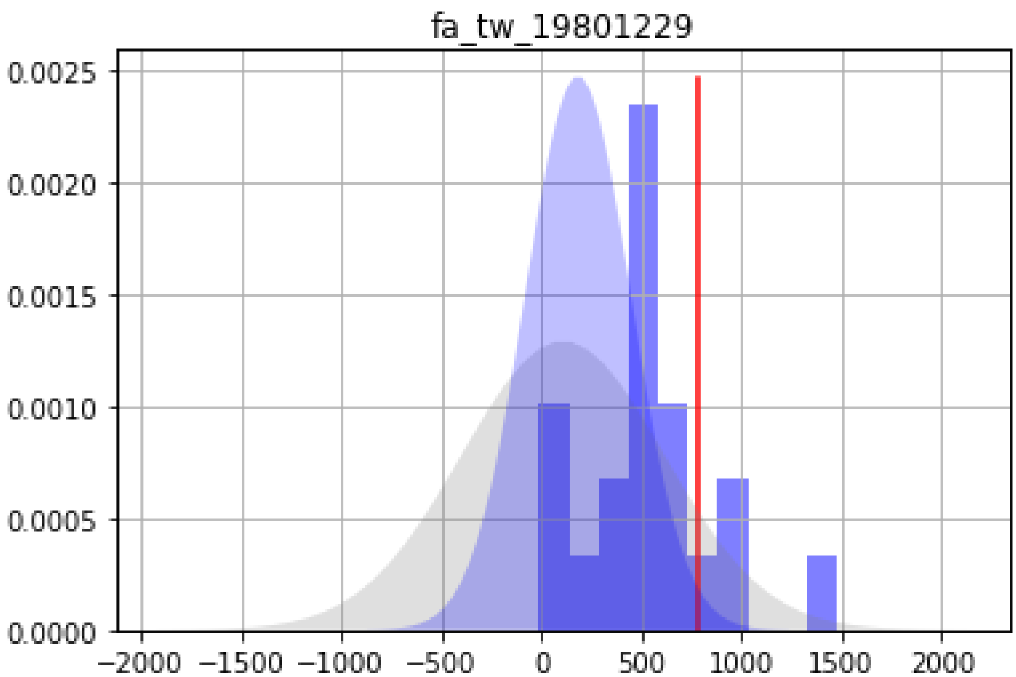
In [29]:

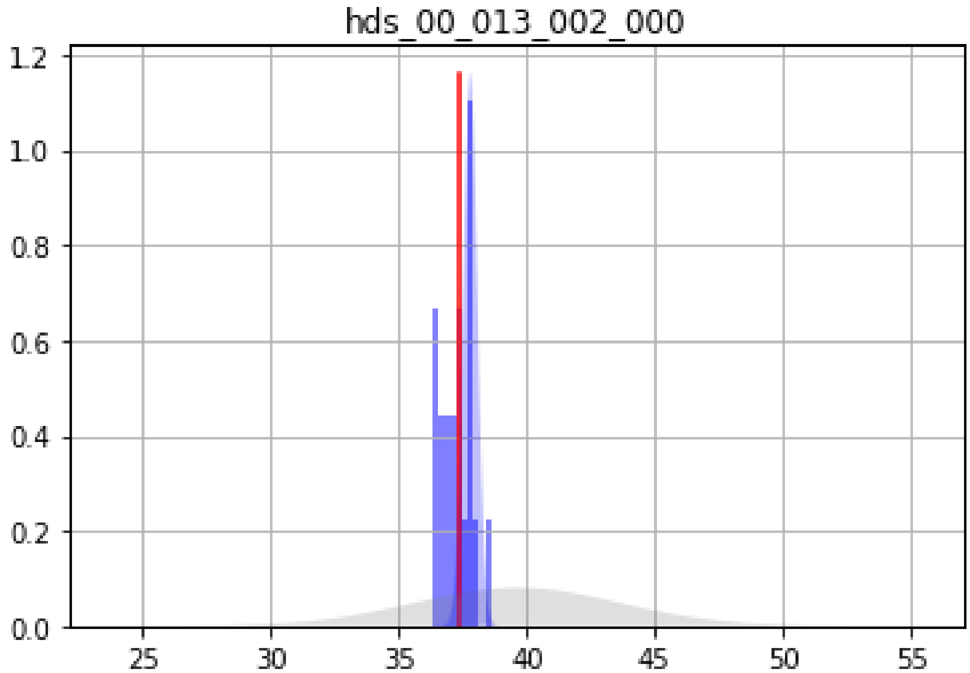
```python
obs = pst.observation_data
fnames = pst.pestpp_options["forecasts"].split(",")
for forecast in fnames:
    ax = plt.subplot(111)
    oe_pt.loc[:,forecast].hist(ax=ax,color="b",alpha=0.5,normed=True)
    ax.plot([obs.loc[forecast,"obsval"],obs.loc[forecast,"obsval"]],ax.get_ylim(),"r")
    axt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

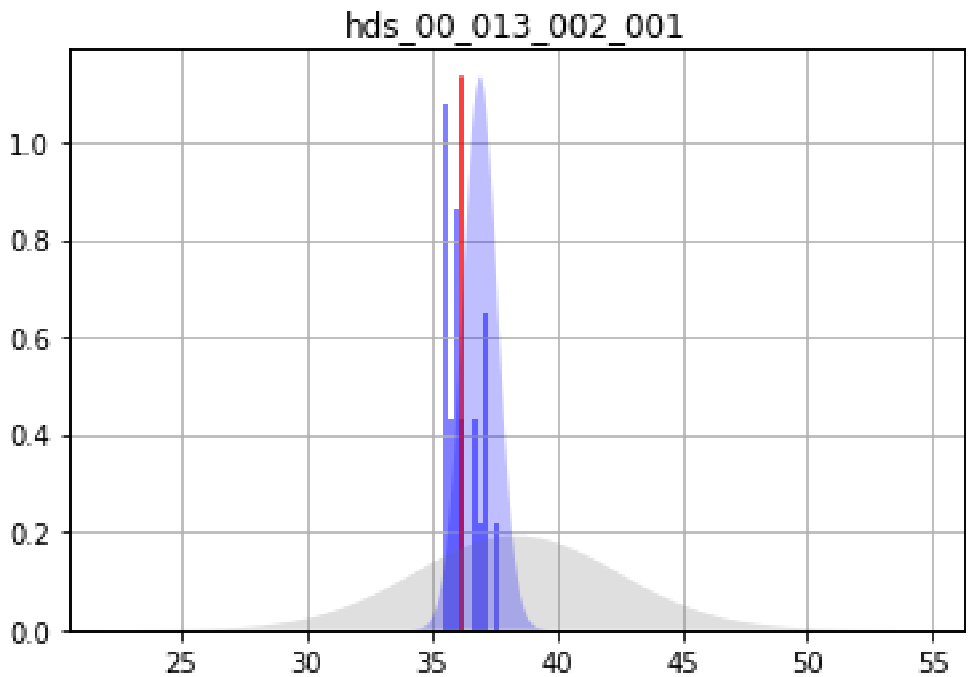

fa_hw_19791230
0.0025
0.0020
0.0015
0.0010
0.0005
0.0000
−2000
−1500
−1000
−500
0

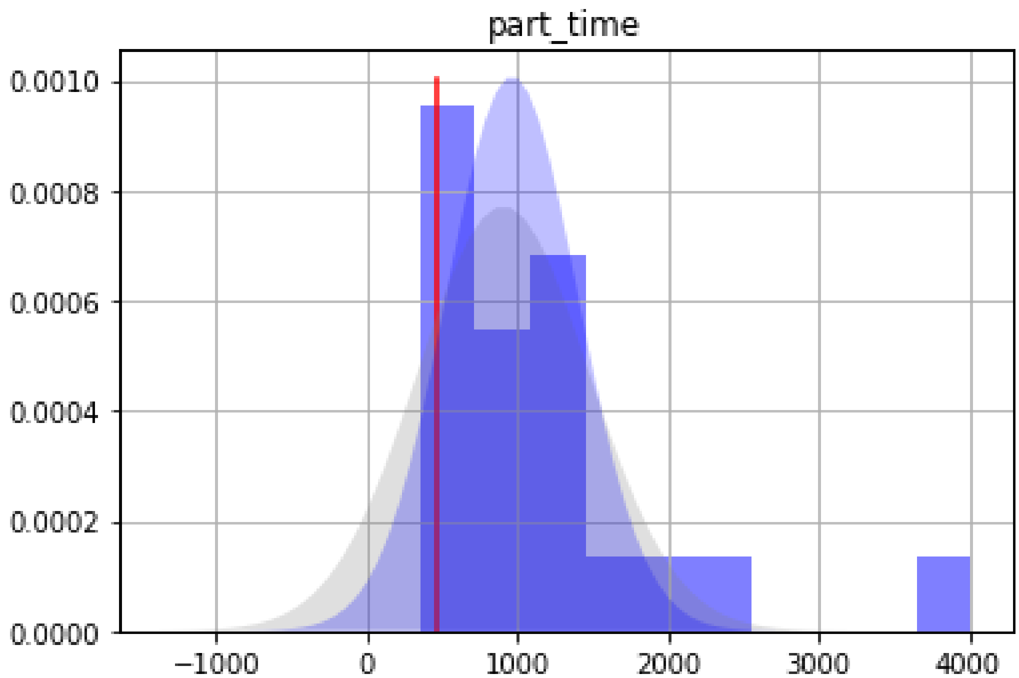

fa_hw_19801229
0.0014
0.0012
0.0010
0.0008
0.0006
0.0004
0.0002
0.0000
−2000
−1500
−1000
−500
0
500
1000
1500

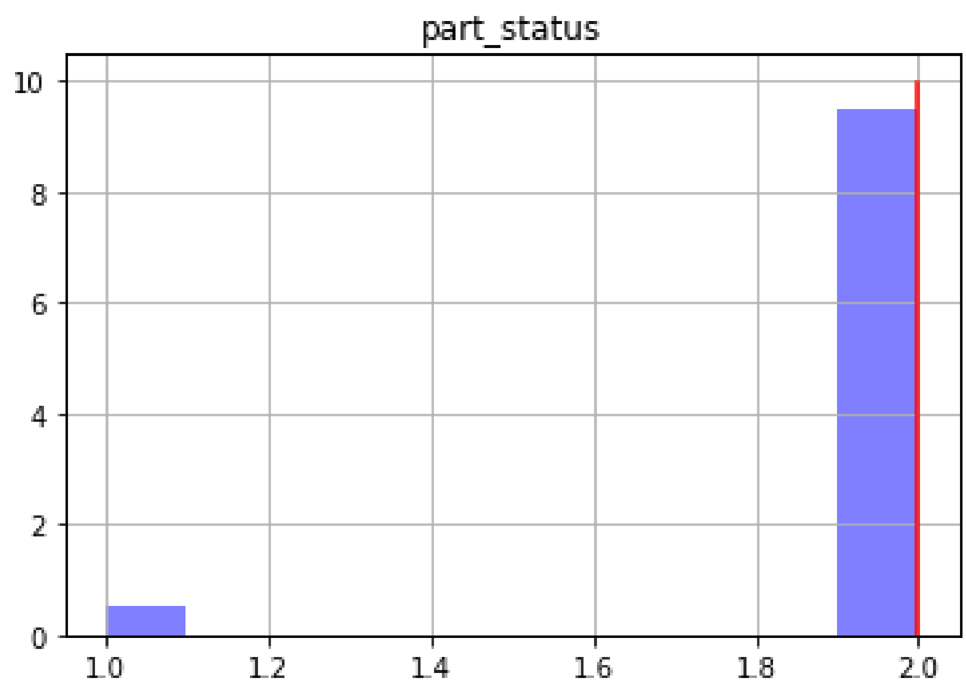

fa_tw_19791230
0.005
0.004
0.003
0.002
0.001
0.000
−2000
−1500
−1000
−500
0
500
1000


fa_tw_19801229
0.0025
0.0020
0.0015
0.0010
0.0005
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
1.0
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
10
8
6
4
2
0
1.0
1.2
1.4
1.6
1.8
2.0