pestpp-glm

May 10, 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_prsity5	gr_prsity5	log	705	0	
pp_rech0	pp_rech0	log	32	0	
gr_vka3	gr_vka3	log	705	0	
gr_ss4	gr_ss4	log	705	0	
cn_rech4	cn_rech4	log	1	0	
cn_hk8	cn_hk8	log	1	0	
strk	strk	log	40	0	
cn_sy7	cn_sy7	log	1	0	
gr_ss3	gr_ss3	log	705	0	
pp_strt0	pp_strt0	log	32	0	
gr_vka4	gr_vka4	log	705	0	

cn_strt8	cn_strt8	log	1	0
drncond_k00	drncond_k00	log	10	0
gr_strt5	gr_strt5	log	705	0
pp_hk1	pp_hk1	log	32	0
gr_prsity3	gr_prsity3	log	705	0
gr_sy5	gr_sy5	log	705	0
cn_ss7	cn_ss7	log	1	0
gr_hk5	gr_hk5	log	705	0
cn_vka6	cn_vka6	log	1	0
gr_rech2	gr_rech2	log	705	0
cn_sy6	cn_sy6	log	1	0
pp_strt1	pp_strt1	log	32	0
cn_vka7	cn_vka7	log	1	0
pp_hk0	pp_hk0	log	32	0
flow	flow	log	1	0
pp_ss2	pp_ss2	log	32	0
cn_prsity8	cn_prsity8	log	1	0
cn_prsity7	cn_prsity7	log	1	0
pp_prsity2	pp_prsity2	log	32	0
...	...	...	...	...
gr_ss5	gr_ss5	log	705	0
gr_sy4	gr_sy4	log	705	0
cn_ss6	cn_ss6	log	1	0
pp_vka2	pp_vka2	log	32	0
cn_hk7	cn_hk7	log	1	0
pp_sy2	pp_sy2	log	32	0
cn_sy8	cn_sy8	log	1	0
gr_strt3	gr_strt3	log	705	0
pp_vka0	pp_vka0	log	32	0
pp_ss1	pp_ss1	log	32	0
cn_ss8	cn_ss8	log	1	0
gr_strt4	gr_strt4	log	705	0
cn_prsity6	cn_prsity6	log	1	0
gr_rech3	gr_rech3	log	705	0
pp_strt2	pp_strt2	log	32	0
welflux	welflux	log	2	0 to 0.176091
cn_strt7	cn_strt7	log	1	0
pp_sy0	pp_sy0	log	32	0
pp_vka1	pp_vka1	log	32	0
cn_strt6	cn_strt6	log	1	0
pp_hk2	pp_hk2	log	32	0
pp_ss0	pp_ss0	log	32	0
gr_hk4	gr_hk4	log	705	0
cn_vka8	cn_vka8	log	1	0
pp_rech1	pp_rech1	log	32	0
pp_prsity0	pp_prsity0	log	32	0
gr_sy3	gr_sy3	log	705	0
cn_rech5	cn_rech5	log	1	-0.39794

pp_sy1	pp_sy1	log	32	0
pp_prsity1	pp_prsity1	log	32	0

	upper bound	lower bound	standard deviation
gr_prsity5	0.176091	-0.30103	0.11928
pp_rech0	0.0413927	-0.0457575	0.0217875
gr_vka3	1	-1	0.5
gr_ss4	1	-1	0.5
cn_rech4	0.0791812	-0.09691	0.0440228
cn_hk8	1	-1	0.5
strk	2	-2	1
cn_sy7	0.243038	-0.60206	0.211275
gr_ss3	1	-1	0.5
pp_strt0	0.0211893	-0.0222764	0.0108664
gr_vka4	1	-1	0.5
cn_strt8	0.0211893	-0.0222764	0.0108664
drncond_k00	1	-1	0.5
gr_strt5	0.0211893	-0.0222764	0.0108664
pp_hk1	1	-1	0.5
gr_prsity3	0.176091	-0.30103	0.11928
gr_sy5	0.243038	-0.60206	0.211275
cn_ss7	1	-1	0.5
gr_hk5	1	-1	0.5
cn_vka6	1	-1	0.5
gr_rech2	0.0413927	-0.0457575	0.0217875
cn_sy6	0.243038	-0.60206	0.211275
pp_strt1	0.0211893	-0.0222764	0.0108664
cn_vka7	1	-1	0.5
pp_hk0	1	-1	0.5
flow	0.09691	-0.124939	0.0554622
pp_ss2	1	-1	0.5
cn_prsity8	0.176091	-0.30103	0.11928
cn_prsity7	0.176091	-0.30103	0.11928
pp_prsity2	0.176091	-0.30103	0.11928
...	...	...	...
gr_ss5	1	-1	0.5
gr_sy4	0.243038	-0.60206	0.211275
cn_ss6	1	-1	0.5
pp_vka2	1	-1	0.5
cn_hk7	1	-1	0.5
pp_sy2	0.243038	-0.60206	0.211275
cn_sy8	0.243038	-0.60206	0.211275
gr_strt3	0.0211893	-0.0222764	0.0108664
pp_vka0	1	-1	0.5
pp_ss1	1	-1	0.5
cn_ss8	1	-1	0.5
gr_strt4	0.0211893	-0.0222764	0.0108664
cn_prsity6	0.176091	-0.30103	0.11928

```
gr_rech3              0.0413927         -0.0457575             0.0217875
pp_strt2              0.0211893         -0.0222764             0.0108664
welflux      0.176091 to 0.30103  -0.30103 to     0  0.0752575 to 0.11928
cn_strt7              0.0211893         -0.0222764             0.0108664
pp_sy0                 0.243038           -0.60206              0.211275
pp_vka1                       1                 -1                   0.5
cn_strt6              0.0211893         -0.0222764             0.0108664
pp_hk2                        1                 -1                   0.5
pp_ss0                        1                 -1                   0.5
gr_hk4                        1                 -1                   0.5
cn_vka8                       1                 -1                   0.5
pp_rech1              0.0413927         -0.0457575             0.0217875
pp_prsity0             0.176091           -0.30103               0.11928
gr_sy3                 0.243038           -0.60206              0.211275
cn_rech5               -0.09691                 -1              0.225772
pp_sy1                 0.243038           -0.60206              0.211275
pp_prsity1             0.176091           -0.30103               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_hk6	1
cn_sy6	1
cn_prsity8	1
cn_rech4	1
cn_hk8	1
cn_strt6	1
cn_ss7	1
cn_ss6	1
cn_strt7	1
cn_vka7	1
cn_sy8	1
flow	1
cn_prsity7	1
cn_sy7	1
cn_vka8	1
cn_prsity6	1
cn_rech5	1
cn_strt8	1
cn_ss8	1
cn_hk7	1
cn_vka6	1
welflux	2
welflux_k02	6
drncond_k00	10
pp_sy0	32
pp_prsity0	32
pp_prsity1	32
pp_strt0	32
pp_sy1	32
pp_strt1	32
pp_strt2	32
pp_vka2	32
pp_ss2	32
pp_prsity2	32
pp_hk1	32
pp_vka0	32
pp_sy2	32
pp_rech0	32

```
pp_ss1          32
pp_hk0          32
pp_hk2          32
pp_ss0          32
pp_vka1         32
pp_rech1        32
strk            40
Name: pargp, dtype: int64
```

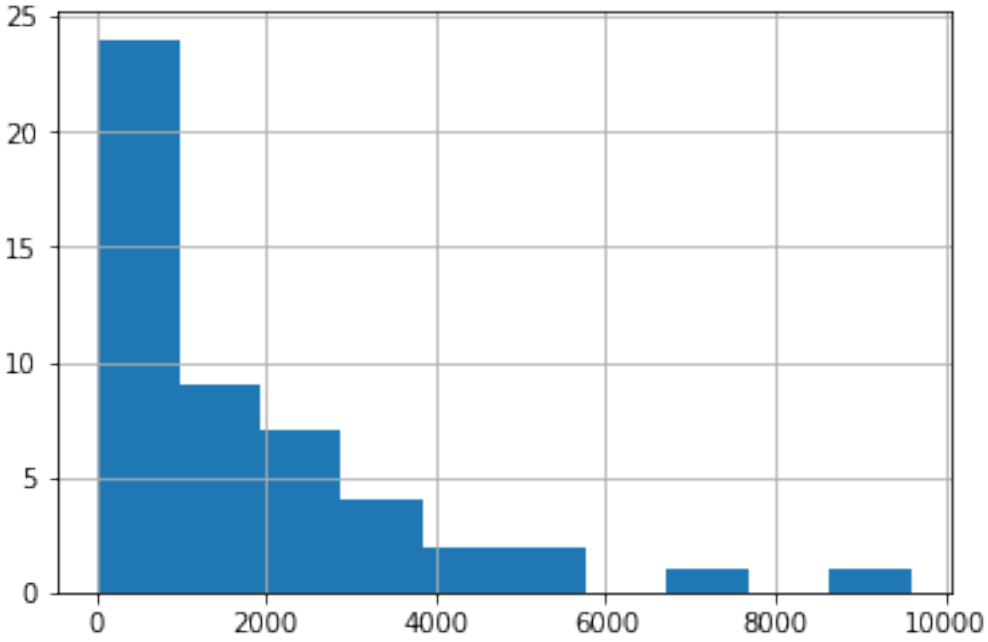
fix the future recharge pilot points, vka in layers 1 and 3 and the initial condition pilot points (we still have layer-scale pars for each of these types)

```
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
         45     19.369533
         34     20.846610
         46     21.882157
         11     22.353237
         49     29.366309
         8      32.918376
```

```
44     41.193909
30     46.635983
10     67.894886
38    121.187577
1     153.424546
29    169.305090
7     197.933663
21    234.861997
35    288.628727
33    296.265990
17    296.719869
41    348.978104
26    523.078249
20    555.670256
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
```

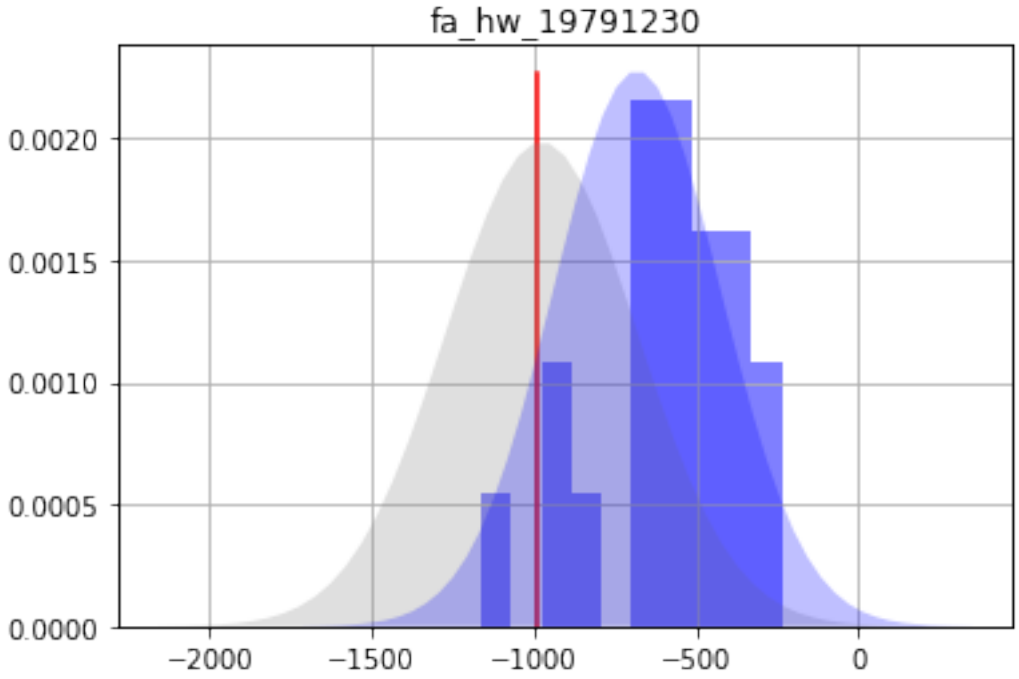
We can also load and plot the FOSM forecast results along side of the ensemble results:

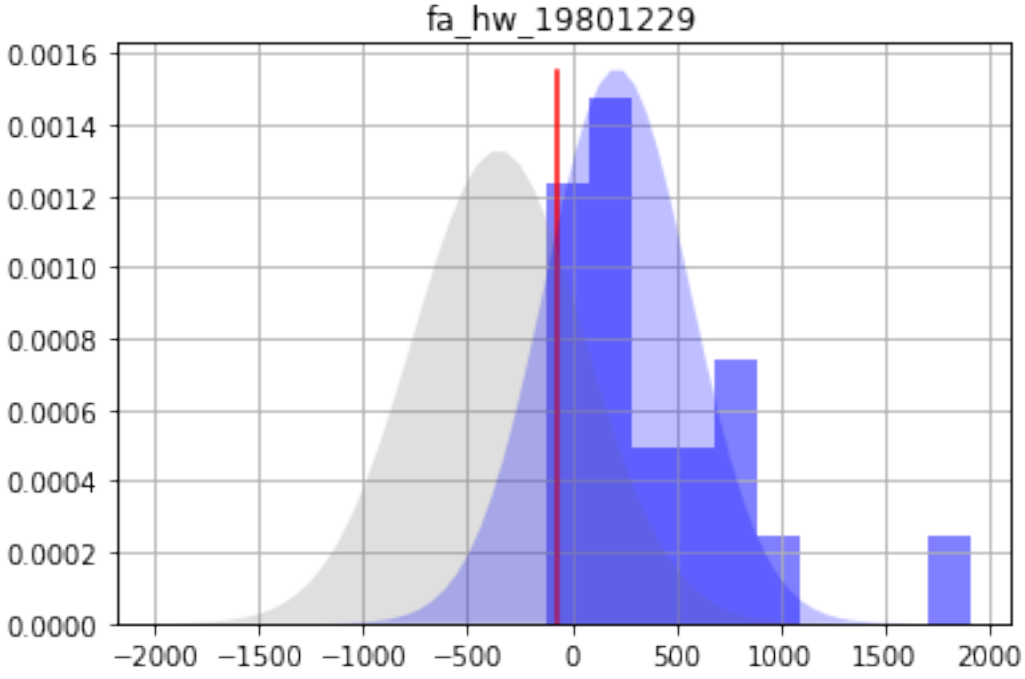
```
In [16]: f_df = pd.read_csv(os.path.join(m_d,"freyberg_pp.pred.usum.csv"),index_col=0)
         f_df.index = f_df.index.map(str.lower)
         f_df
```

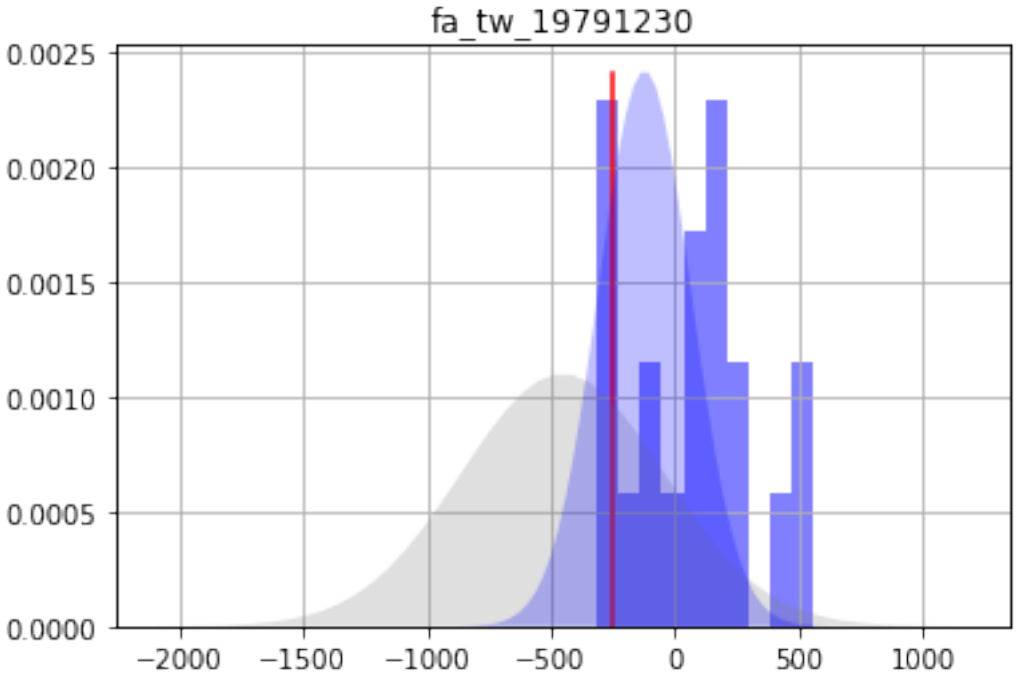
Out[16]:

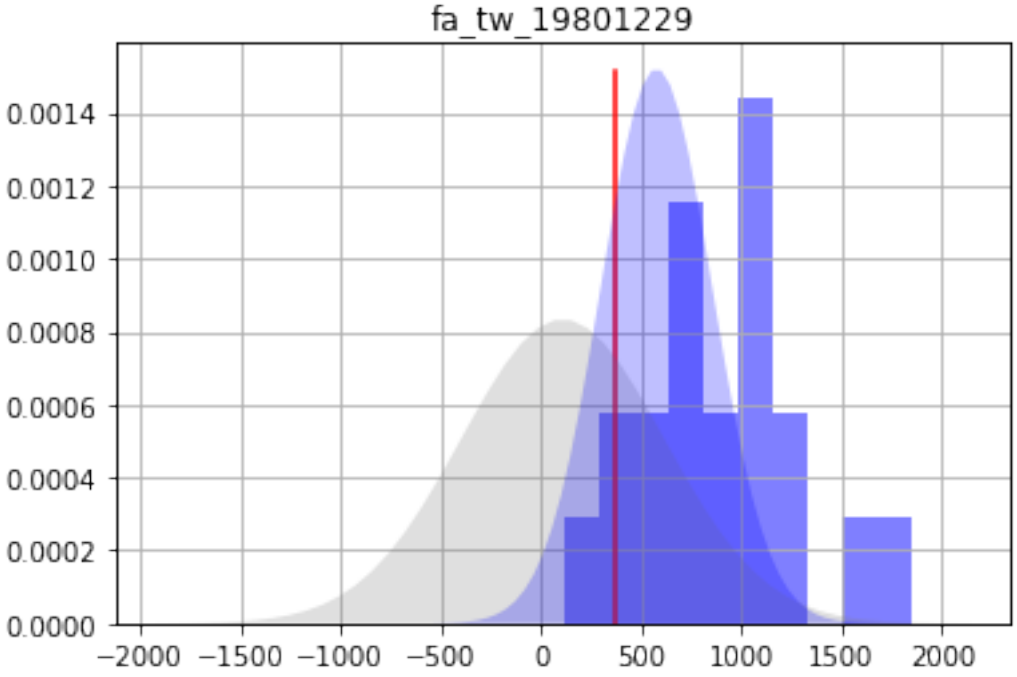
name	prior_mean	prior_stdev	prior_lower_bound	prior_upper_bound	post_mean	post_stdev	post_lower_bound	post_upper_bound
fa_hw_19791230	-977.2390	295.32800	-1567.8900	-386.5840	-683.0780	257.446000	-1197.9700	-168.1850
fa_hw_19801229	-351.2160	409.77000	-1170.7600	468.3240	216.9670	349.390000	-481.8120	915.7460
fa_tw_19791230	-453.0330	409.35100	-1271.7400	365.6690	-122.8870	185.967000	-494.8220	249.0480
fa_tw_19801229	108.9600	506.73200	-904.5040	1122.4200	577.0510	277.727000	21.5971	1132.5100
hds_00_013_002_000	39.6102	3.96314	31.6840	47.5365	35.6590	0.371793	34.9155	36.4026
hds_00_013_002_001	38.3838	4.05782	30.2681	46.4994	34.7388	0.731605	33.2756	36.2020
part_status	2.0000	0.00000	2.0000	2.0000	1.0000	0.000000	1.0000	1.0000
part_time	907.7020	570.98600	-234.2690	2049.6700	4015.0000	443.065000	3128.8700	4901.1300

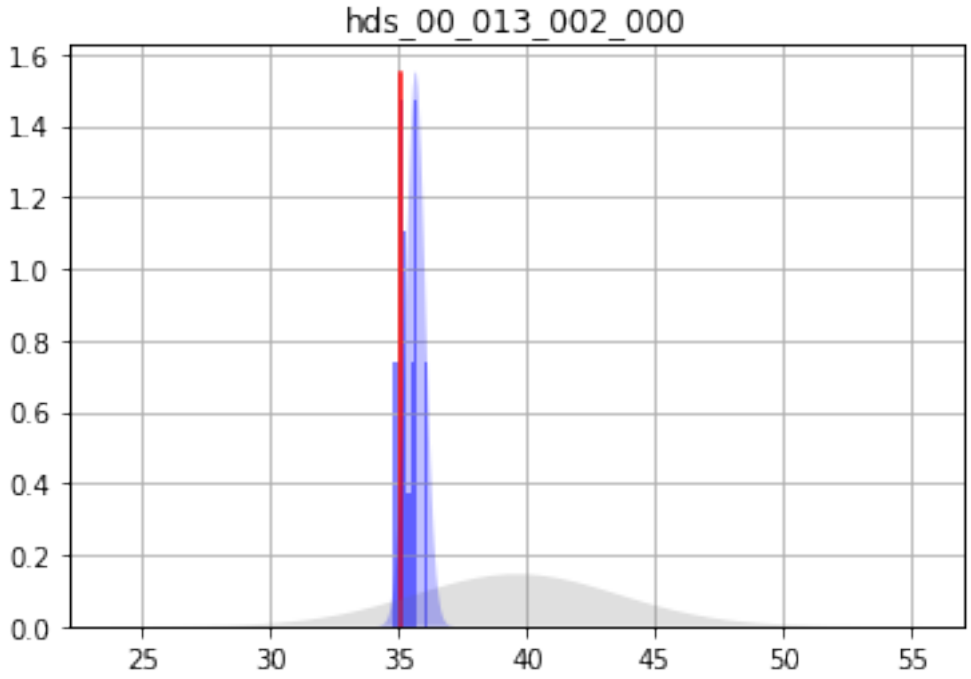
In [17]:
```
obs = pst.observation_data
fnames = pst.pestpp_options["forecasts"].split(",")
for forecast in fnames:
    ax = plt.subplot(111)
    oe_pt.loc[:,forecast].hist(ax=ax,color="b",alpha=0.5,normed=True)
    ax.plot([obs.loc[forecast,"obsval"],obs.loc[forecast,"obsval"]],ax.get_ylim(),"r"
  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

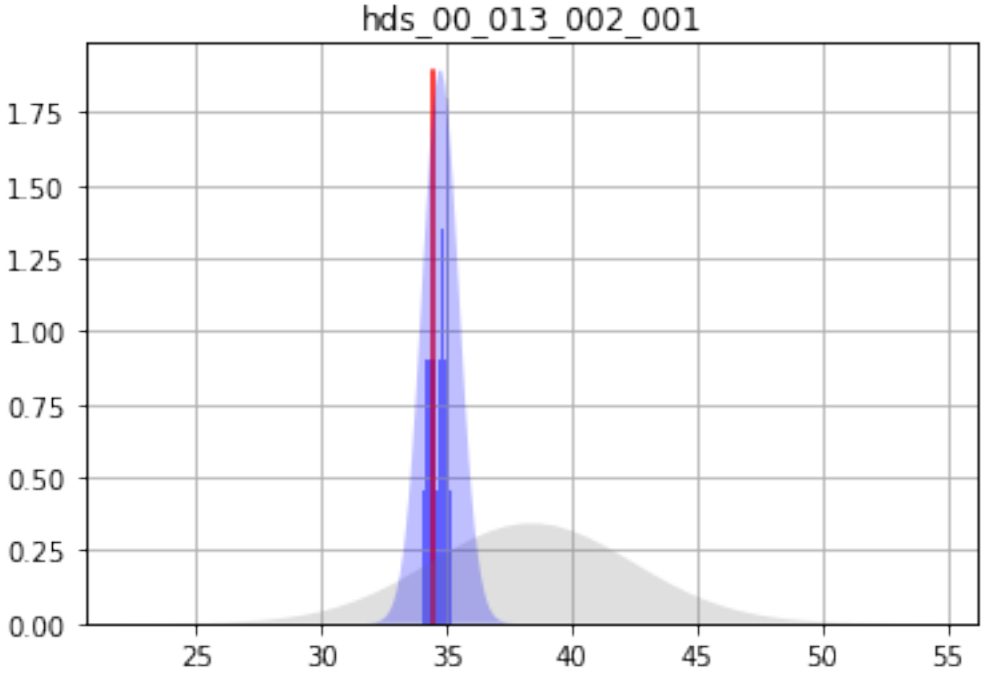

fa_hw_19791230
0.0020
0.0015
0.0010
0.0005
0.0000
−2000
−1500
−1000
−500
0

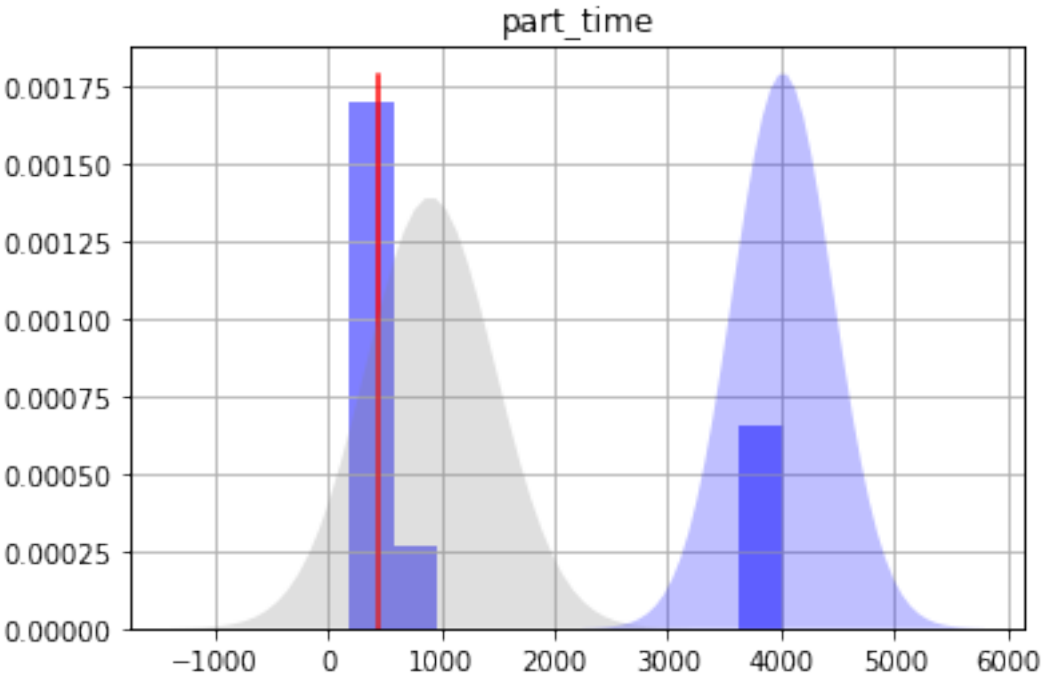

fa_hw_19801229
0.0016
0.0014
0.0012
0.0010
0.0008
0.0006
0.0004
0.0002
0.0000
−2000
−1500
−1000
−500
0
500
1000
1500
2000

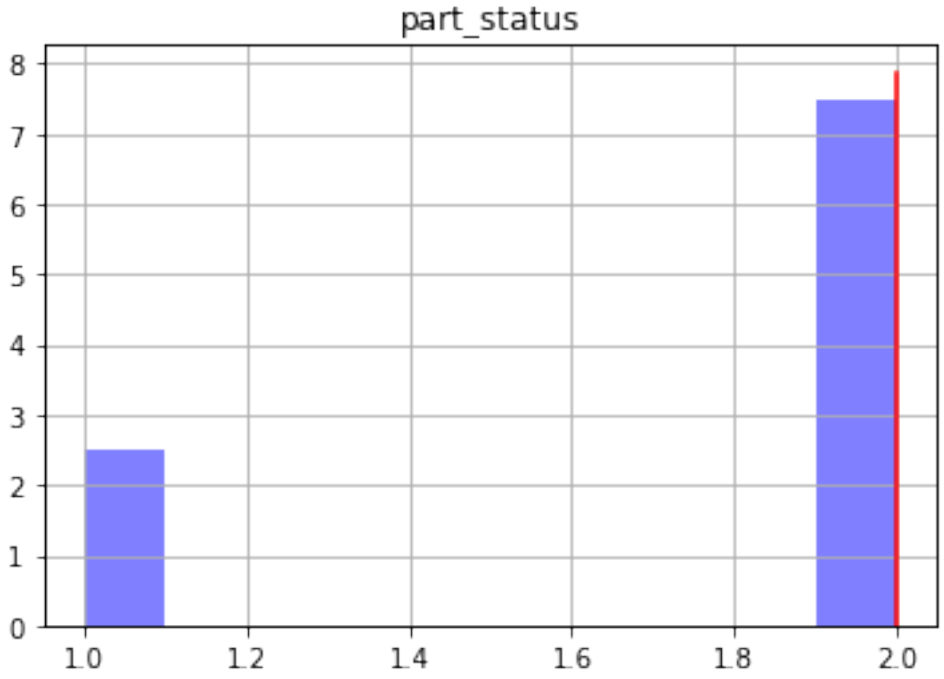

fa_tw_19791230
0.0025
0.0020
0.0015
0.0010
0.0005
0.0000
−2000
−1500
−1000
−500
0
500
1000


fa_tw_19801229
0.0014
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
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


hds_00_013_002_001
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
0.00175
0.00150
0.00125
0.00100
0.00075
0.00050
0.00025
0.00000
−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'
```

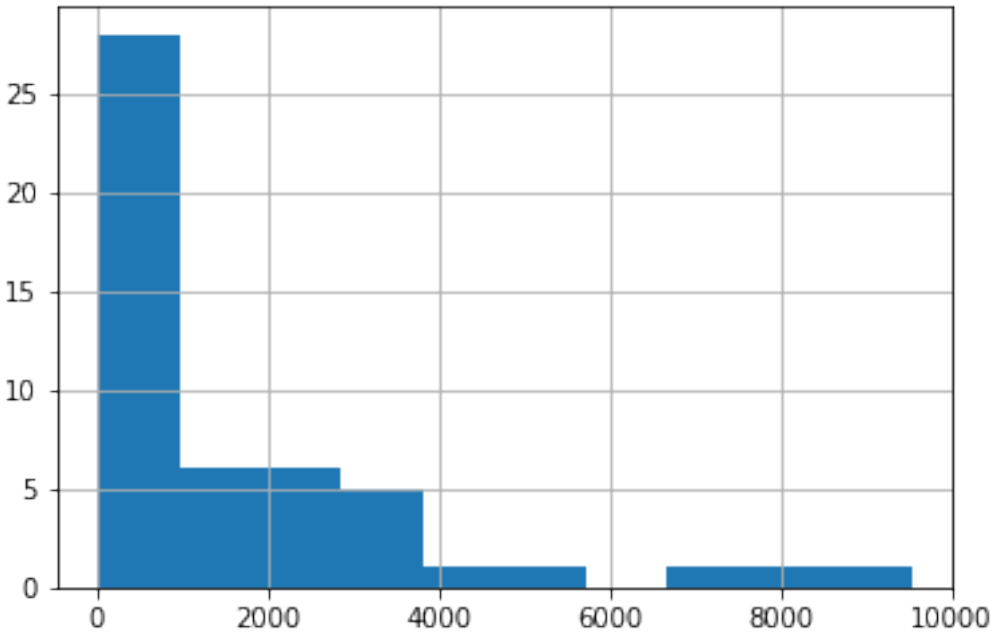
```
In [22]: pst.pestpp_options["base_jacobian"] = "restart_pp.jcb"
         pst.reg_data.phimlim = pst.nnz_obs
         pst.reg_data.phimaccept = pst.reg_data.phimlim * 1.1
         pst.write(os.path.join(t_d,"freyberg_pp.pst"))
```

```
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_ro
                                    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
         49     12.211321
         45     44.197023
         11     70.946143
         34     72.128879
         20     80.509778
         46    114.542769
         44    134.483626
         17    154.613525
         10    163.211140
         35    170.024936
         30    170.247477
         41    216.605116
         37    293.688548
         47    324.709679
         7     344.635389
         40    403.592937
         1     408.648229
         8     430.019036
         13    448.043824
         21    456.891746
         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],:]
```

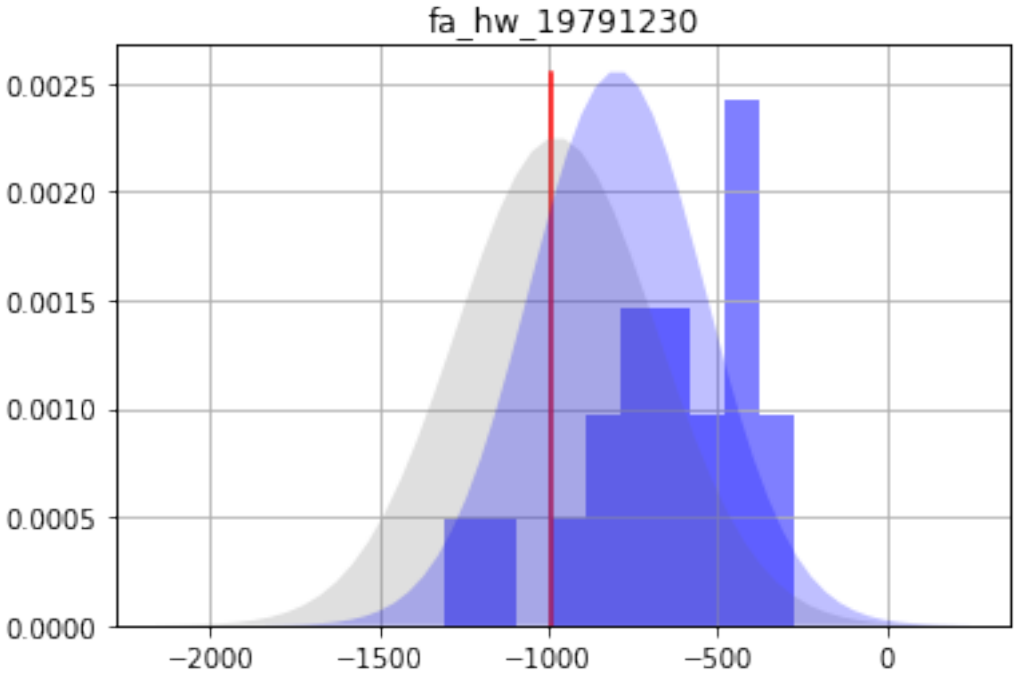
```
In [27]: f_df = pd.read_csv(os.path.join(m_d,"freyberg_pp.pred.usum.csv"),index_col=0)
         f_df.index = f_df.index.map(str.lower)
         f_df
```

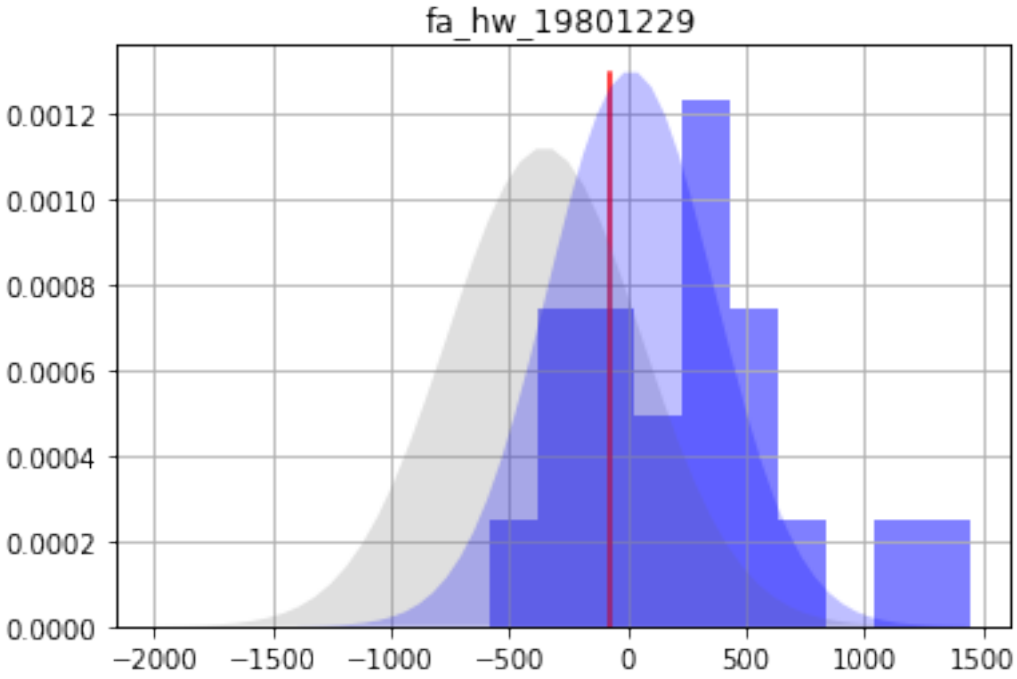
Out[27]:

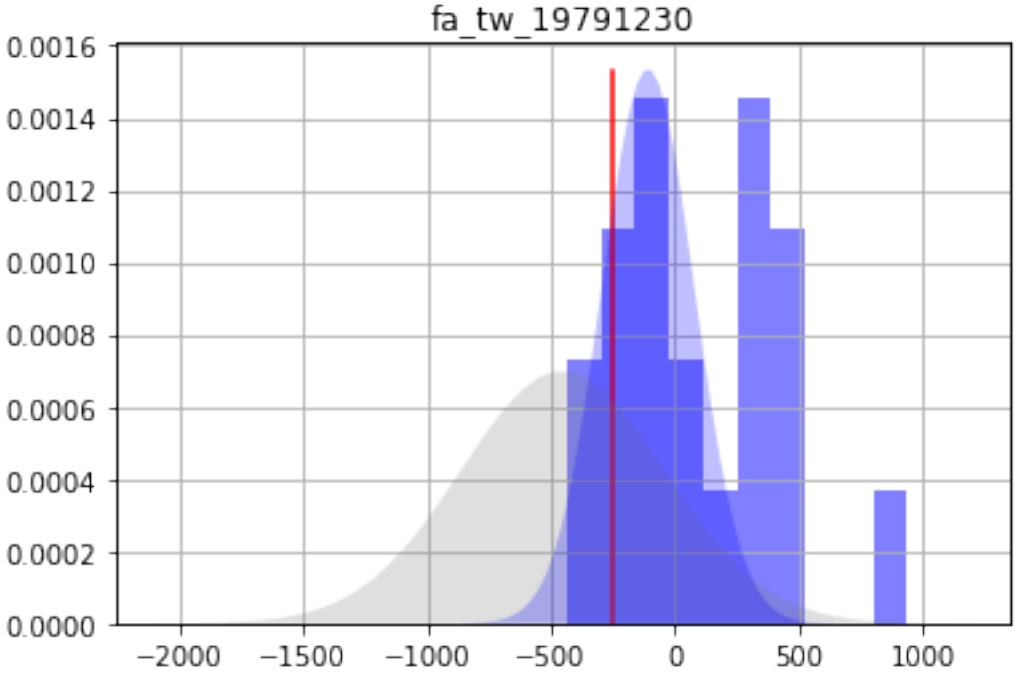
	prior_mean	prior_stdev	prior_lower_bound	prior_upper_bound	post_mean	post_stdev	post_lower_bound	post_upper_bound
name								
fa_hw_19791230	-977.2390	295.32800	-1567.8900	-386.5840	-797.5000	259.781000	-1317.06000	-277.9390
fa_hw_19801229	-351.2160	409.77000	-1170.7600	468.3240	15.1497	353.117000	-691.08300	721.3830
fa_tw_19791230	-453.0330	409.35100	-1271.7400	365.6690	-109.3180	186.415000	-482.14700	263.5120
fa_tw_19801229	108.9600	506.73200	-904.5040	1122.4200	562.1340	277.838000	6.45674	1117.8100
hds_00_013_002_000	39.6102	3.96314	31.6840	47.5365	35.9870	0.462778	35.06140	36.9125
hds_00_013_002_001	38.3838	4.05782	30.2681	46.4994	34.9912	0.779721	33.43180	36.5507
part_status	2.0000	0.00000	2.0000	2.0000	1.0000	0.000000	1.00000	1.0000
part_time	907.7020	570.98600	-234.2690	2049.6700	4015.0000	443.279000	3128.44000	4901.5600

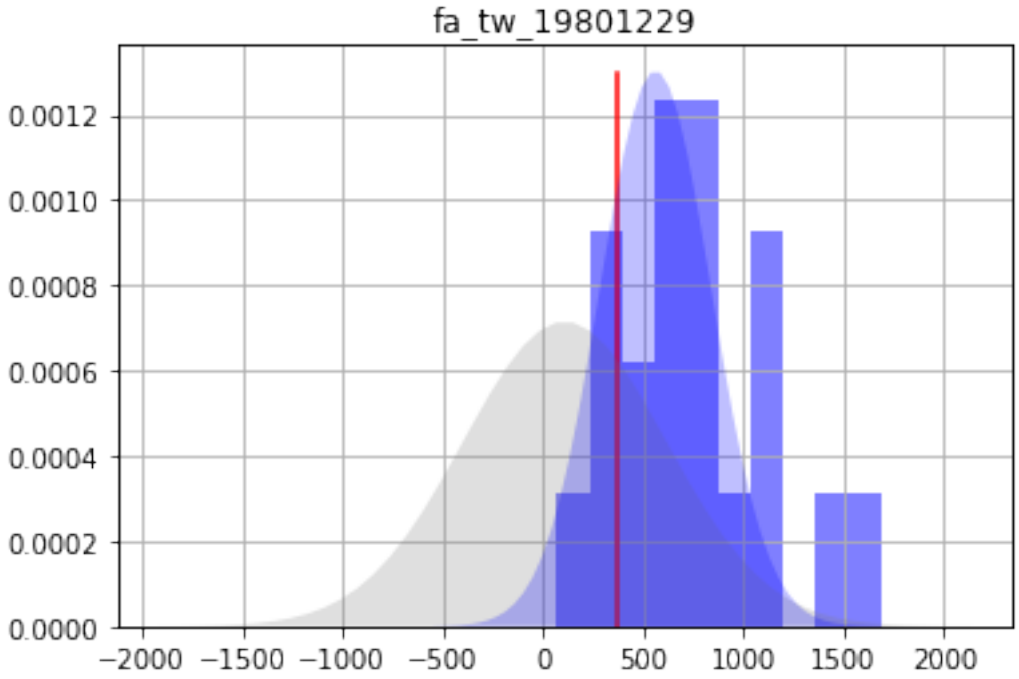
```
In [28]: obs = pst.observation_data
         fnames = pst.pestpp_options["forecasts"].split(",")
         for forecast in fnames:
             ax = plt.subplot(111)
             oe_pt.loc[:,forecast].hist(ax=ax,color="b",alpha=0.5,normed=True)
             ax.plot([obs.loc[forecast,"obsval"],obs.loc[forecast,"obsval"]],ax.get_ylim(),"r"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

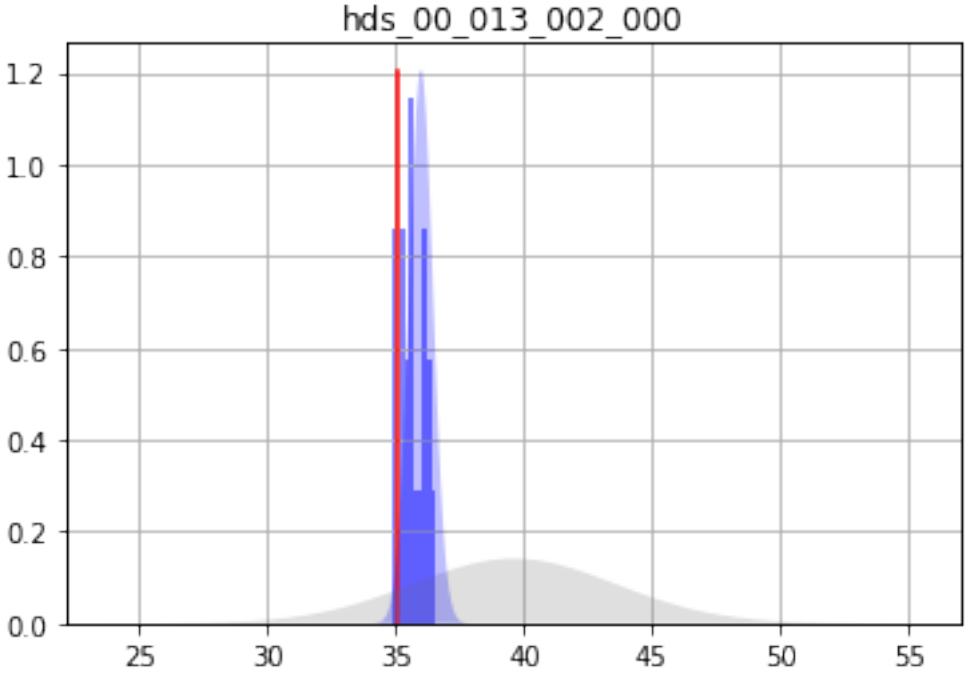
```
x,y = pyemu.plot_utils.gaussian_distribution(f_df.loc[forecast,"prior_mean"],f_df
axt.fill_between(x,0,y,facecolor="0.5",alpha=0.25)
x,y = pyemu.plot_utils.gaussian_distribution(f_df.loc[forecast,"post_mean"],f_df.
axt.fill_between(x,0,y,facecolor="b",alpha=0.25)
axt.set_ylim(0,axt.get_ylim()[1])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

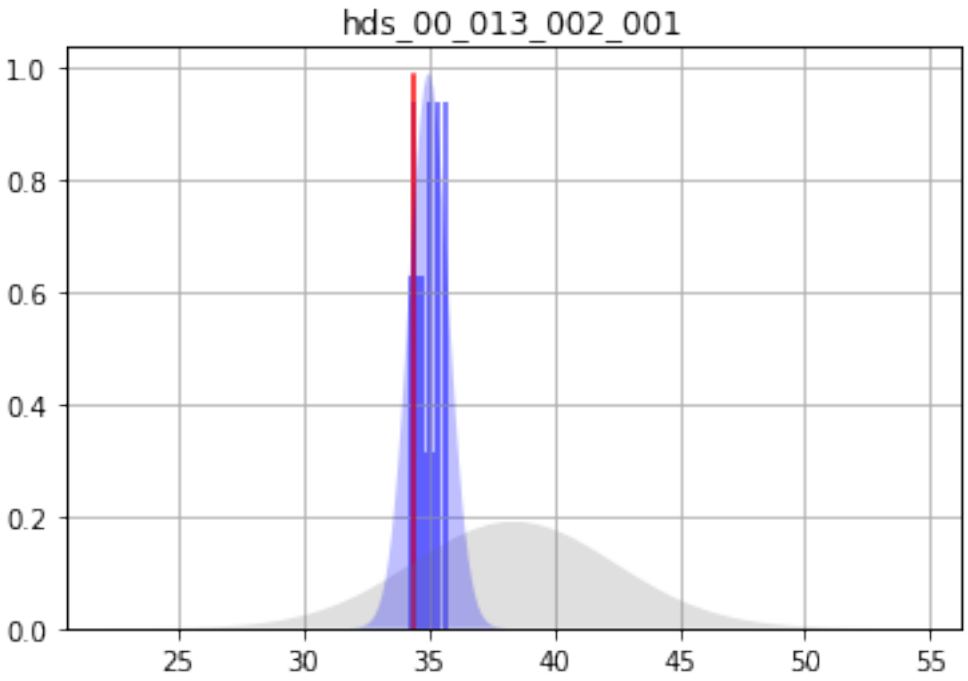


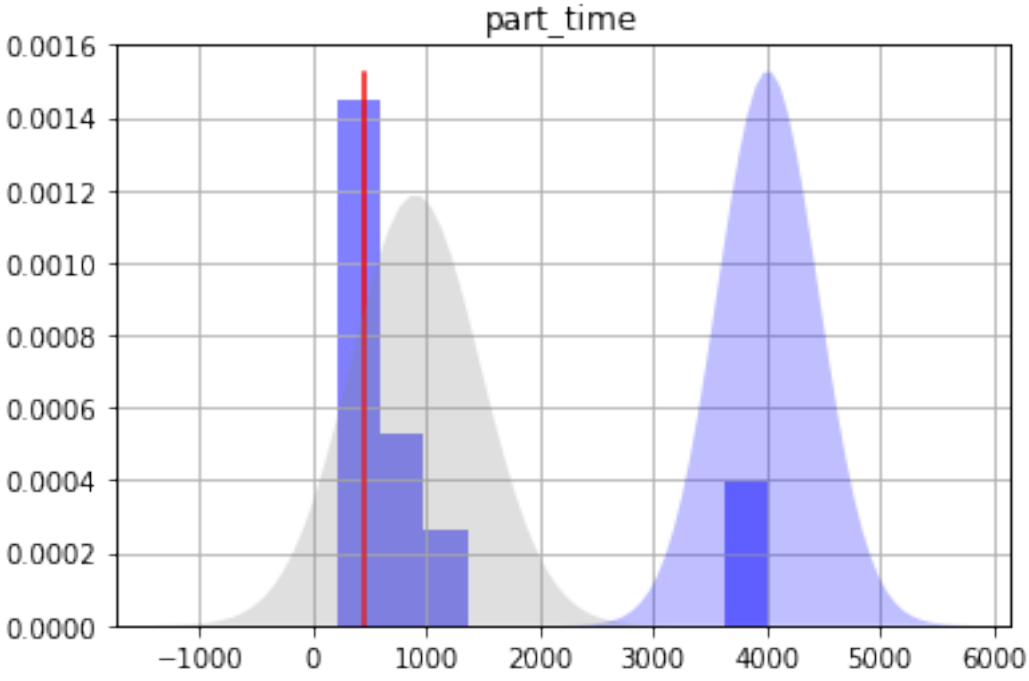

fa_hw_19801229
0.0012
0.0010
0.0008
0.0006
0.0004
0.0002
0.0000
−2000
−1500
−1000
−500
0
500
1000
1500

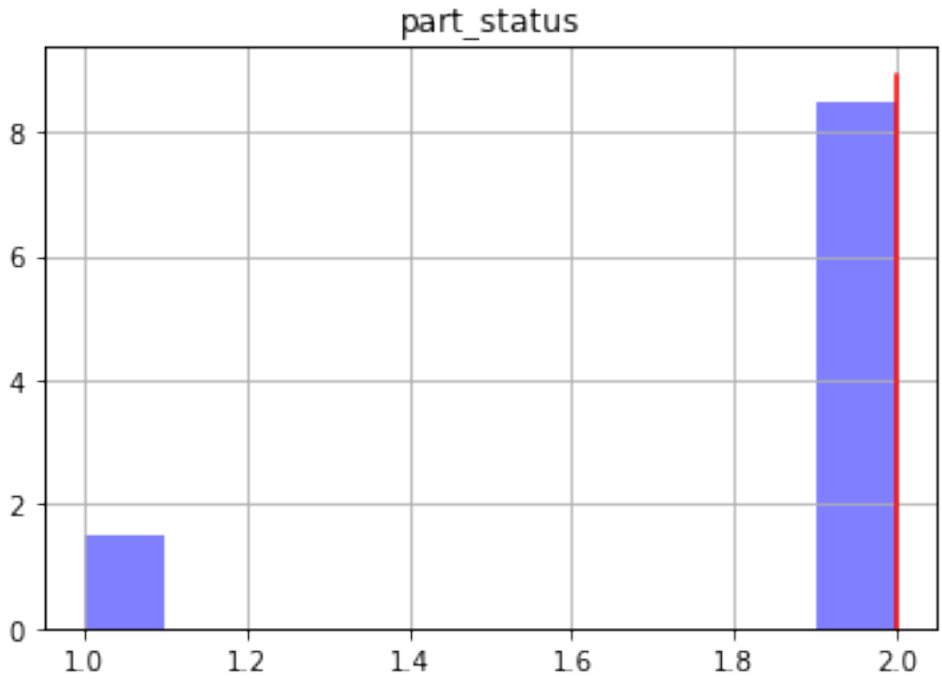

fa_tw_19791230
0.0016
0.0014
0.0012
0.0010
0.0008
0.0006
0.0004
0.0002
0.0000
−2000
−1500
−1000
−500
0
500
1000


fa_tw_19801229
0.0012
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
1.0
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
5000
6000


part_status
8
6
4
2
0
1.0
1.2
1.4
1.6
1.8
2.0