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	\
strk	strk	log	40	0	
cn_sy8	cn_sy8	log	1	0	
gr_ss4	gr_ss4	log	705	0	
gr_ss3	gr_ss3	log	705	0	
pp_vka2	pp_vka2	log	32	0	
cn_strt7	cn_strt7	log	1	0	
gr_rech3	gr_rech3	log	705	0	
cn_prsity7	cn_prsity7	log	1	0	
gr_prsity3	gr_prsity3	log	705	0	
cn_rech4	cn_rech4	log	1	0	
gr_vka5	gr_vka5	log	705	0	

pp_sy0	pp_sy0	log	32	0
cn_hk6	cn_hk6	log	1	0
pp_ss1	pp_ss1	log	32	0
cn_rech5	cn_rech5	log	1	-0.39794
cn_strt6	cn_strt6	log	1	0
gr_strt5	gr_strt5	log	705	0
gr_sy3	gr_sy3	log	705	0
cn_hk7	cn_hk7	log	1	0
gr_prsity4	gr_prsity4	log	705	0
cn_ss7	cn_ss7	log	1	0
cn_prsity8	cn_prsity8	log	1	0
cn_prsity6	cn_prsity6	log	1	0
pp_strt2	pp_strt2	log	32	0
cn_vka6	cn_vka6	log	1	0
pp_ss2	pp_ss2	log	32	0
pp_strt1	pp_strt1	log	32	0
gr_hk5	gr_hk5	log	705	0
cn_hk8	cn_hk8	log	1	0
gr_sy5	gr_sy5	log	705	0
...	...	...	...	...
gr_strt4	gr_strt4	log	705	0
gr_sy4	gr_sy4	log	705	0
cn_sy7	cn_sy7	log	1	0
pp_strt0	pp_strt0	log	32	0
pp_hk1	pp_hk1	log	32	0
pp_hk0	pp_hk0	log	32	0
cn_strt8	cn_strt8	log	1	0
gr_hk4	gr_hk4	log	705	0
pp_vka1	pp_vka1	log	32	0
gr_ss5	gr_ss5	log	705	0
cn_ss6	cn_ss6	log	1	0
pp_ss0	pp_ss0	log	32	0
cn_vka7	cn_vka7	log	1	0
welflux	welflux	log	2	0 to 0.176091
gr_prsity5	gr_prsity5	log	705	0
gr_vka4	gr_vka4	log	705	0
pp_rech0	pp_rech0	log	32	0
cn_sy6	cn_sy6	log	1	0
pp_prsity0	pp_prsity0	log	32	0
pp_rech1	pp_rech1	log	32	0
gr_hk3	gr_hk3	log	705	0
pp_vka0	pp_vka0	log	32	0
pp_prsity1	pp_prsity1	log	32	0
welflux_k02	welflux_k02	log	6	0
gr_vka3	gr_vka3	log	705	0
cn_ss8	cn_ss8	log	1	0
pp_hk2	pp_hk2	log	32	0
flow	flow	log	1	0

pp_prsity2	pp_prsity2	log	32	0	
pp_sy1	pp_sy1	log	32	0	

	upper bound	lower bound	standard deviation
strk	2	-2	1
cn_sy8	0.243038	-0.60206	0.211275
gr_ss4	1	-1	0.5
gr_ss3	1	-1	0.5
pp_vka2	1	-1	0.5
cn_strt7	0.0211893	-0.0222764	0.0108664
gr_rech3	0.0413927	-0.0457575	0.0217875
cn_prsity7	0	-1	0.25
gr_prsity3	0	-1	0.25
cn_rech4	0.0791812	-0.09691	0.0440228
gr_vka5	1	-1	0.5
pp_sy0	0.243038	-0.60206	0.211275
cn_hk6	1	-1	0.5
pp_ss1	1	-1	0.5
cn_rech5	-0.09691	-1	0.225772
cn_strt6	0.0211893	-0.0222764	0.0108664
gr_strt5	0.0211893	-0.0222764	0.0108664
gr_sy3	0.243038	-0.60206	0.211275
cn_hk7	1	-1	0.5
gr_prsity4	0	-1	0.25
cn_ss7	1	-1	0.5
cn_prsity8	0	-1	0.25
cn_prsity6	0	-1	0.25
pp_strt2	0.0211893	-0.0222764	0.0108664
cn_vka6	1	-1	0.5
pp_ss2	1	-1	0.5
pp_strt1	0.0211893	-0.0222764	0.0108664
gr_hk5	1	-1	0.5
cn_hk8	1	-1	0.5
gr_sy5	0.243038	-0.60206	0.211275
...	...	...	...
gr_strt4	0.0211893	-0.0222764	0.0108664
gr_sy4	0.243038	-0.60206	0.211275
cn_sy7	0.243038	-0.60206	0.211275
pp_strt0	0.0211893	-0.0222764	0.0108664
pp_hk1	1	-1	0.5
pp_hk0	1	-1	0.5
cn_strt8	0.0211893	-0.0222764	0.0108664
gr_hk4	1	-1	0.5
pp_vka1	1	-1	0.5
gr_ss5	1	-1	0.5
cn_ss6	1	-1	0.5
pp_ss0	1	-1	0.5
cn_vka7	1	-1	0.5

```
welflux      0.176091 to 0.30103  -0.30103 to     0  0.0752575 to 0.11928
gr_prsity5                     0                -1                  0.25
gr_vka4                        1                -1                   0.5
pp_rech0               0.0413927        -0.0457575             0.0217875
cn_sy6                  0.243038          -0.60206              0.211275
pp_prsity0                     0                -1                  0.25
pp_rech1               0.0413927        -0.0457575             0.0217875
gr_hk3                         1                -1                   0.5
pp_vka0                        1                -1                   0.5
pp_prsity1                     0                -1                  0.25
welflux_k02                    1                -1                   0.5
gr_vka3                        1                -1                   0.5
cn_ss8                         1                -1                   0.5
pp_hk2                         1                -1                   0.5
flow                     0.09691         -0.124939             0.0554622
pp_prsity2                     0                -1                  0.25
pp_sy1                  0.243038          -0.60206              0.211275

[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_strt6        1
cn_hk7          1
cn_rech4        1
cn_rech5        1
cn_hk6          1
cn_strt7        1
cn_prsity8      1
cn_ss7          1
cn_prsity6      1
cn_vka6         1
cn_ss8          1
cn_hk8          1
cn_prsity7      1
cn_vka8         1
cn_sy7          1
cn_strt8        1
cn_ss6          1
cn_vka7         1
cn_sy6          1
flow            1
welflux         2
welflux_k02     6
drncond_k00    10
pp_hk0         32
pp_sy1         32
pp_vka1        32
pp_strt2       32
pp_ss2         32
pp_prsity2     32
pp_ss1         32
pp_sy0         32
pp_sy2         32
pp_hk2         32
pp_hk1         32
pp_strt0       32
pp_vka0        32
pp_rech0       32
```

```
pp_strt1       32
pp_vka2        32
pp_prsity0     32
pp_rech1       32
pp_ss0         32
pp_prsity1     32
strk           40
Name: pargp, dtype: int64
```

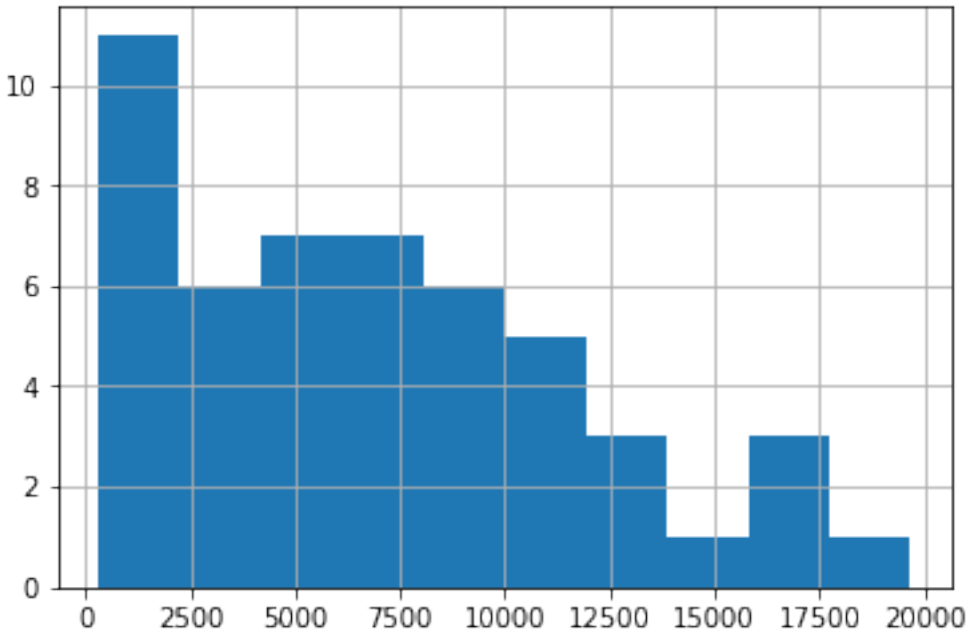
fix the future recharge pilot points, vka in layers 1 and 3 and the initial condition pilot points (we still have layer-scale pars for each of these types)

```
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
         40     300.402885
         45     555.407952
         6      697.909767
         9      717.298349
         11     782.518726
         20     905.929630
         42     936.951440
         21     979.176592
         49    1188.282724
```

```
41    1956.268550
25    2165.826653
22    3247.541258
1     3382.082289
39    3890.602707
24    3939.673160
33    3942.549541
8     4024.830575
15    4408.586314
35    4425.374021
29    4828.066923
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
```

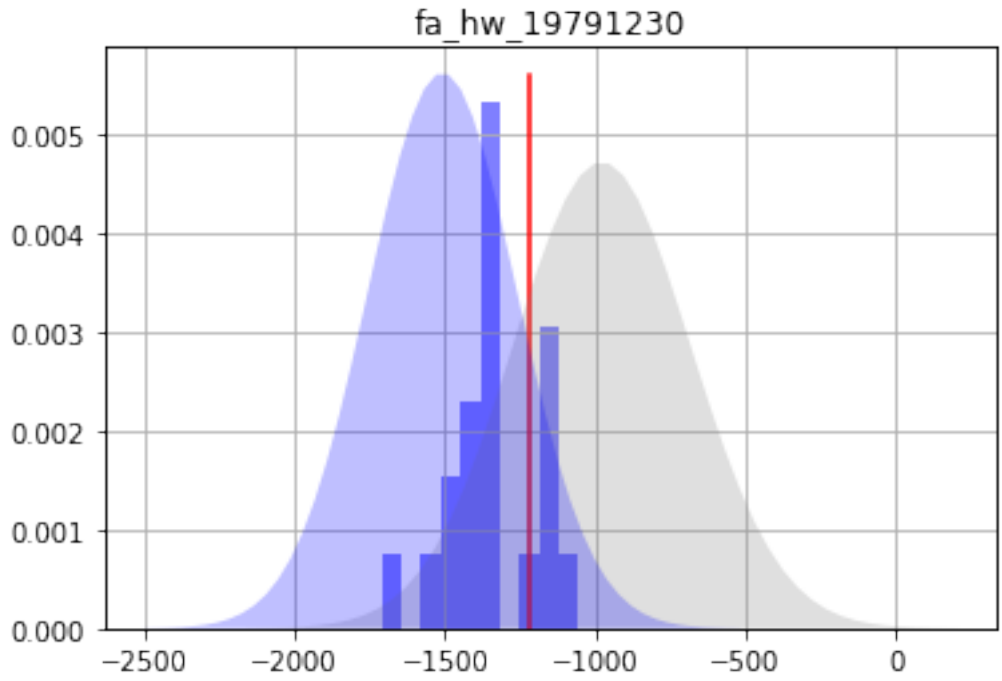
We can also load and plot the FOSM forecast results along side of the ensemble results:

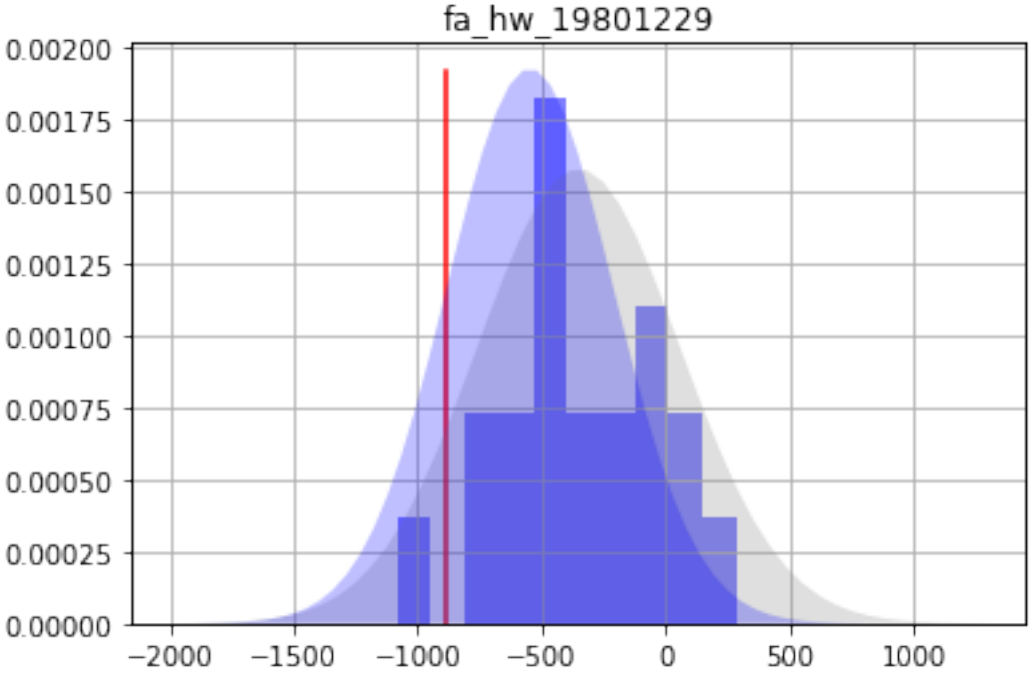
```
In [16]: f_df = pd.read_csv(os.path.join(m_d,"freyberg_pp.pred.usum.csv"),index_col=0)
         f_df.index = f_df.index.map(str.lower)
         f_df
```

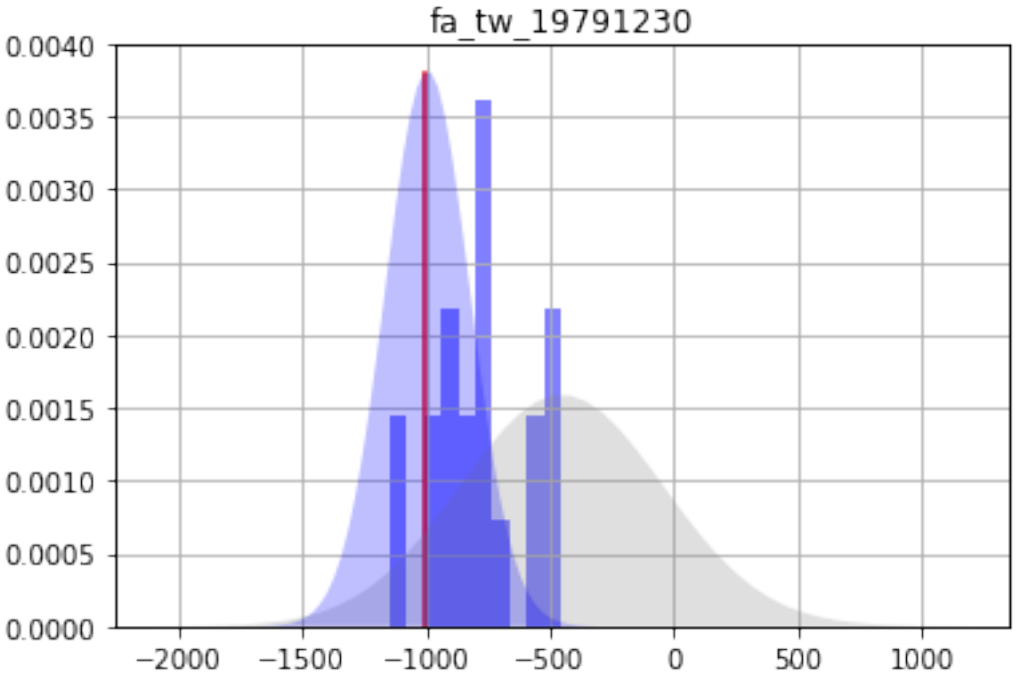
```
Out[16]:                    prior_mean  prior_stdev  prior_lower_bound  \
         name
```

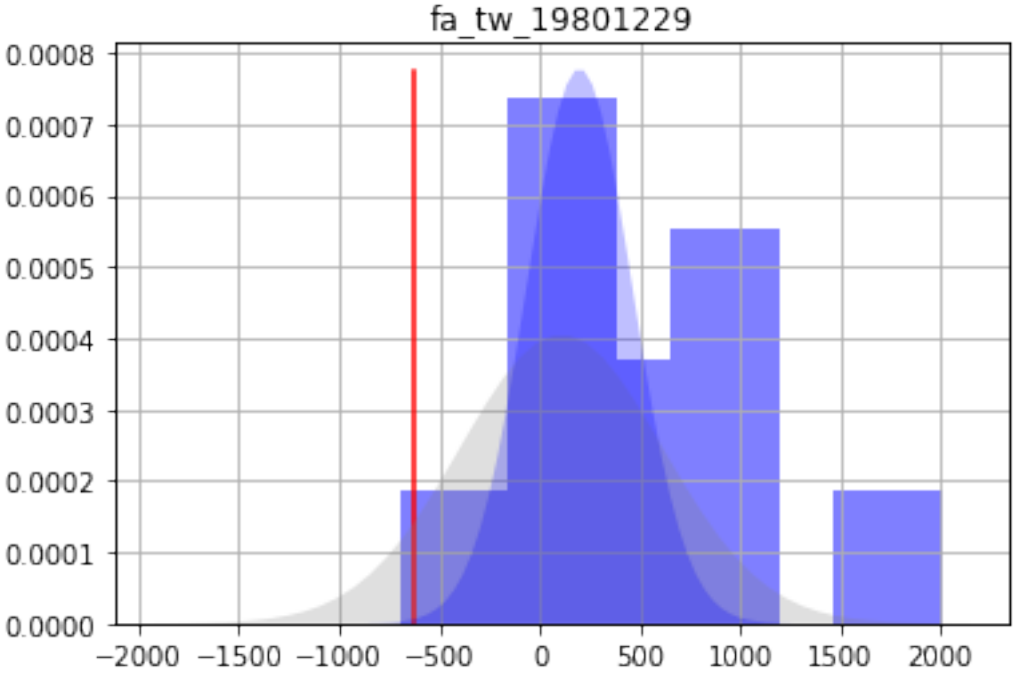
```
fa_hw_19791230       -977.2390    295.32800         -1567.8900
fa_hw_19801229       -351.2160    409.77000         -1170.7600
fa_tw_19791230       -453.0330    409.35100         -1271.7400
fa_tw_19801229        108.9600    506.73200          -904.5040
hds_00_013_002_000     39.6102      3.96314            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 -1507.1700  247.835000
fa_hw_19801229               468.3240  -547.7180  335.549000
fa_tw_19791230               365.6690  -993.5230  170.577000
fa_tw_19801229              1122.4200   199.5300  263.671000
hds_00_013_002_000            47.5365    44.5738    0.273990
hds_00_013_002_001            46.4994    41.0369    0.687833
part_status                    2.0000     2.0000    0.000000
part_time                   2317.2000  1131.0700  601.307000

                    post_lower_bound  post_upper_bound
name
fa_hw_19791230           -2002.8500        -1011.5000
fa_hw_19801229           -1218.8200          123.3800
fa_tw_19791230           -1334.6800         -652.3690
fa_tw_19801229            -327.8120          726.8720
hds_00_013_002_000          44.0258           45.1218
hds_00_013_002_001          39.6612           42.4125
part_status                  2.0000            2.0000
part_time                  -71.5422         2333.6900
```

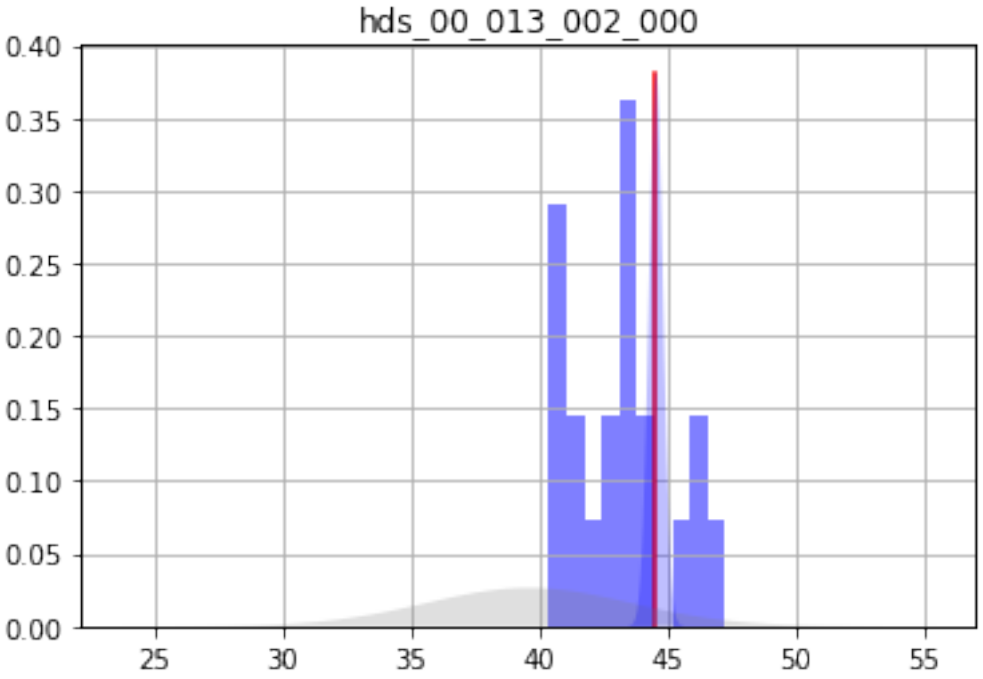
In [17]:
```
obs = pst.observation_data
fnames = pst.pestpp_options["forecasts"].split(",")
for forecast in fnames:
    ax = plt.subplot(111)
    oe_pt.loc[:,forecast].hist(ax=ax,color="b",alpha=0.5,normed=True)
    ax.plot([obs.loc[forecast,"obsval"],obs.loc[forecast,"obsval"]],ax.get_ylim(),"r"
  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

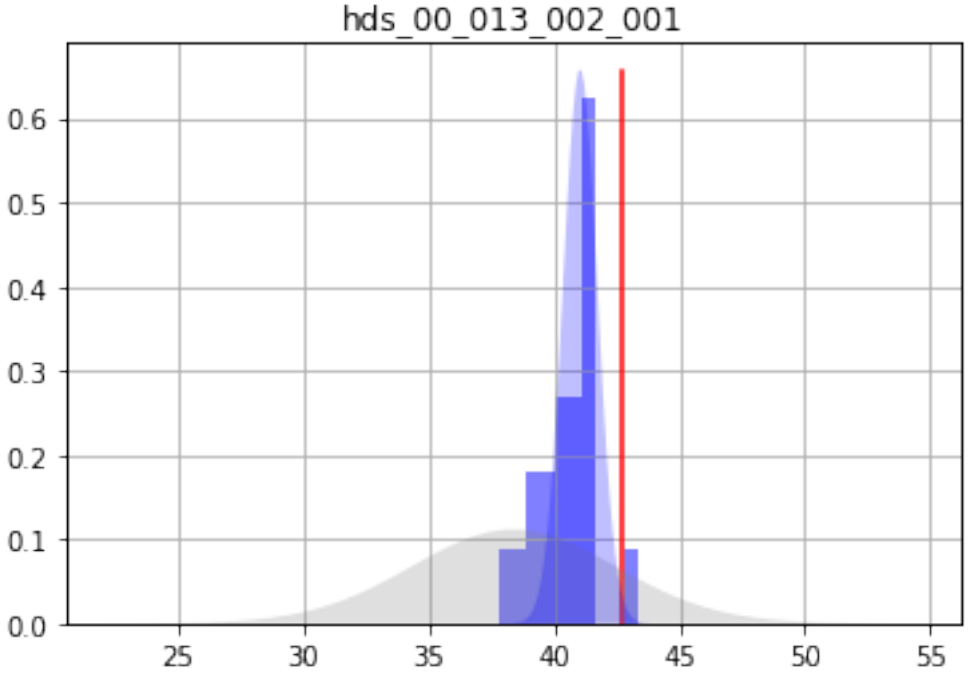

fa_hw_19791230
0.005
0.004
0.003
0.002
0.001
0.000
−2500
−2000
−1500
−1000
−500
0

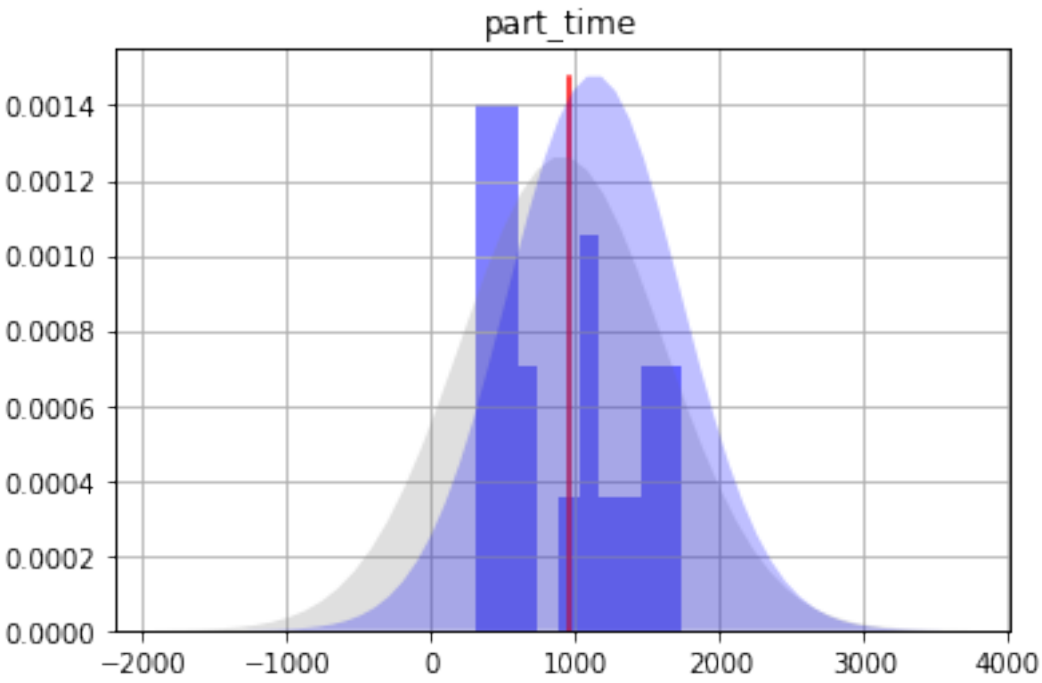

fa_hw_19801229
0.00200
0.00175
0.00150
0.00125
0.00100
0.00075
0.00050
0.00025
0.00000
−2000
−1500
−1000
−500
0
500
1000

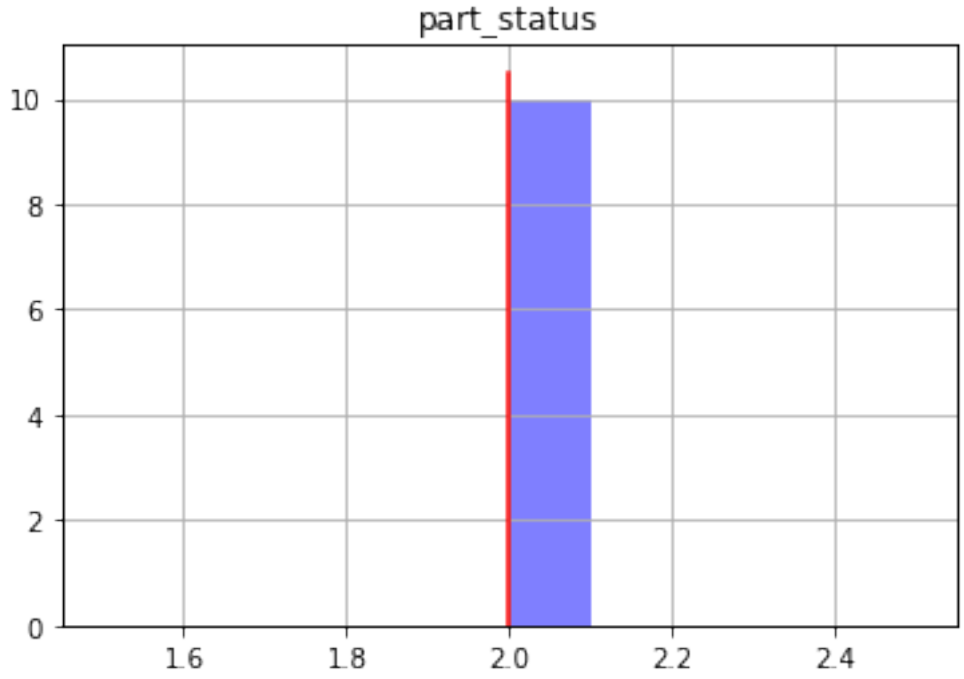

fa_tw_19791230
0.0040
0.0035
0.0030
0.0025
0.0020
0.0015
0.0010
0.0005
0.0000
−2000
−1500
−1000
−500
0
500
1000


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
0.40
0.35
0.30
0.25
0.20
0.15
0.10
0.05
0.00
25
30
35
40
45
50
55


hds_00_013_002_001
0.6
0.5
0.4
0.3
0.2
0.1
0.0
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
−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

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'
```

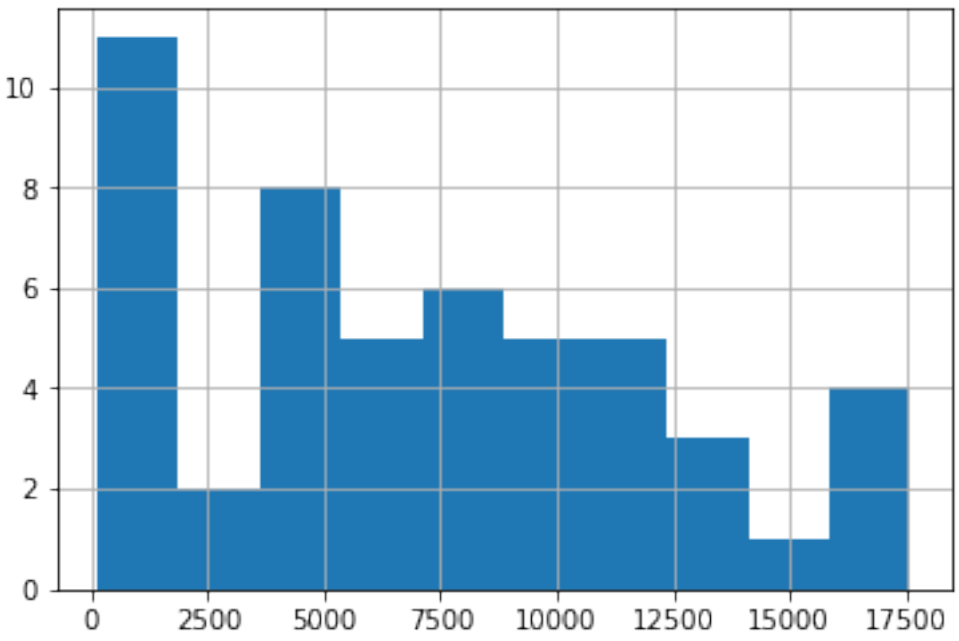
```
In [22]: pst.pestpp_options["base_jacobian"] = "restart_pp.jcb"
         pst.reg_data.phimlim = pst.nnz_obs
         pst.reg_data.phimaccept = pst.reg_data.phimlim * 1.1
         pst.write(os.path.join(t_d,"freyberg_pp.pst"))
```

```
In [23]: pyemu.os_utils.start_slaves(t_d,"pestpp-glm","freyberg_pp.pst",num_slaves=20,slave_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
         45     123.370340
         21     397.421709
         42     726.315210
         11     757.015238
         12     760.083645
         22     954.707091
         6      986.267185
         9     1165.488353
         24    1255.508405
         1     1267.298833
         19    1636.716287
         40    2396.789452
         20    3502.906187
         49    3845.532325
         47    3915.474869
         25    4190.860266
         26    4238.373573
         41    4349.334208
         8     4434.012635
         23    4541.078978
         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],:]
```

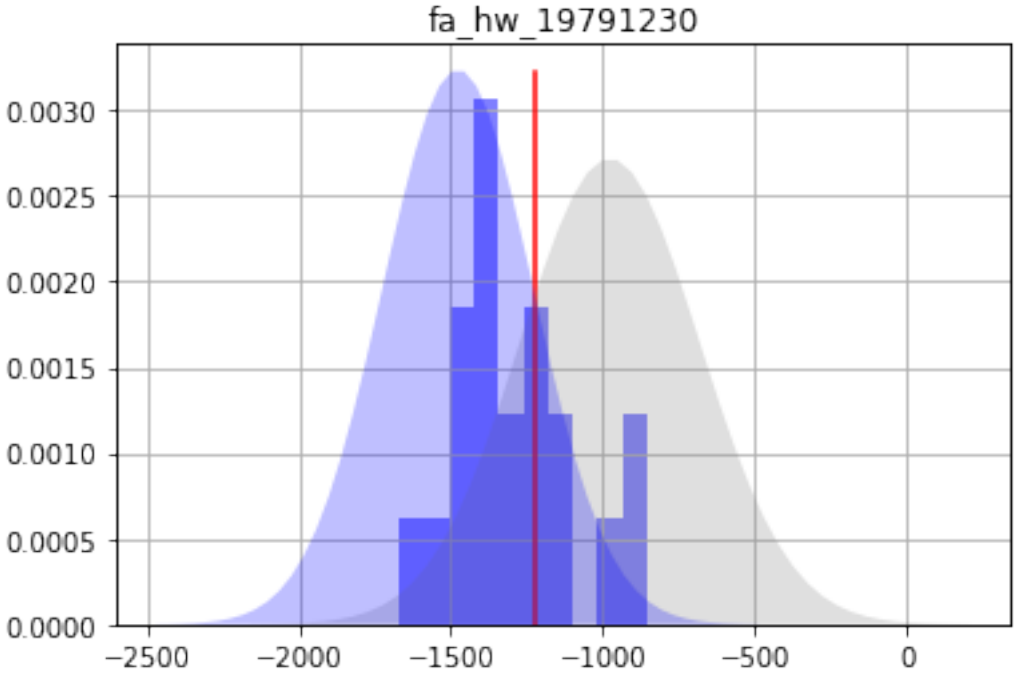
In [27]:
```
f_df = pd.read_csv(os.path.join(m_d,"freyberg_pp.pred.usum.csv"),index_col=0)
f_df.index = f_df.index.map(str.lower)
f_df
```

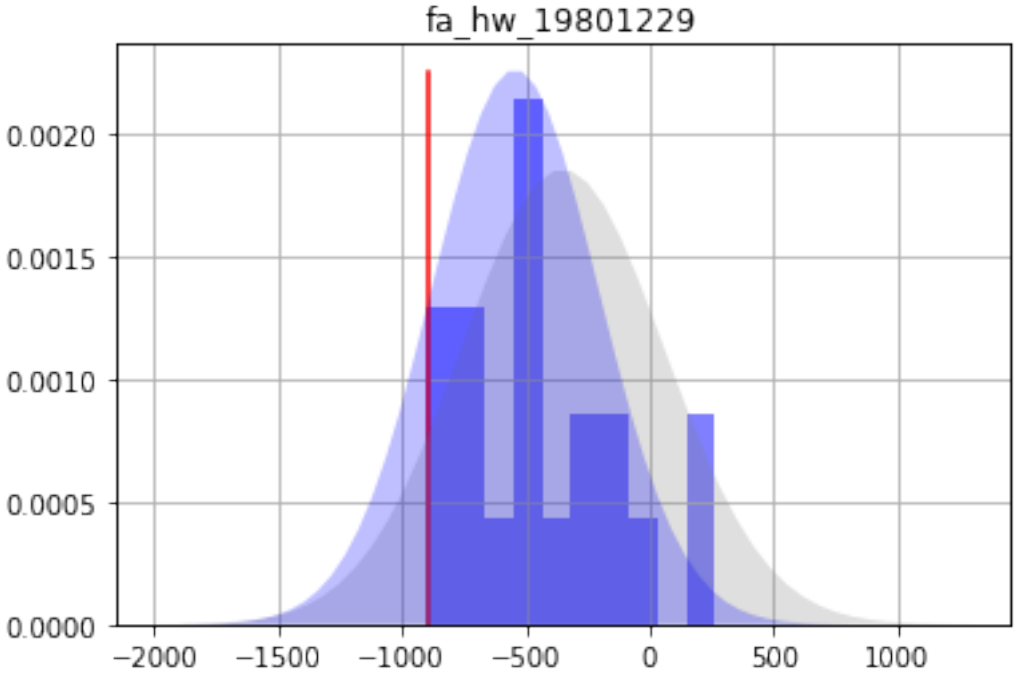
Out[27]:

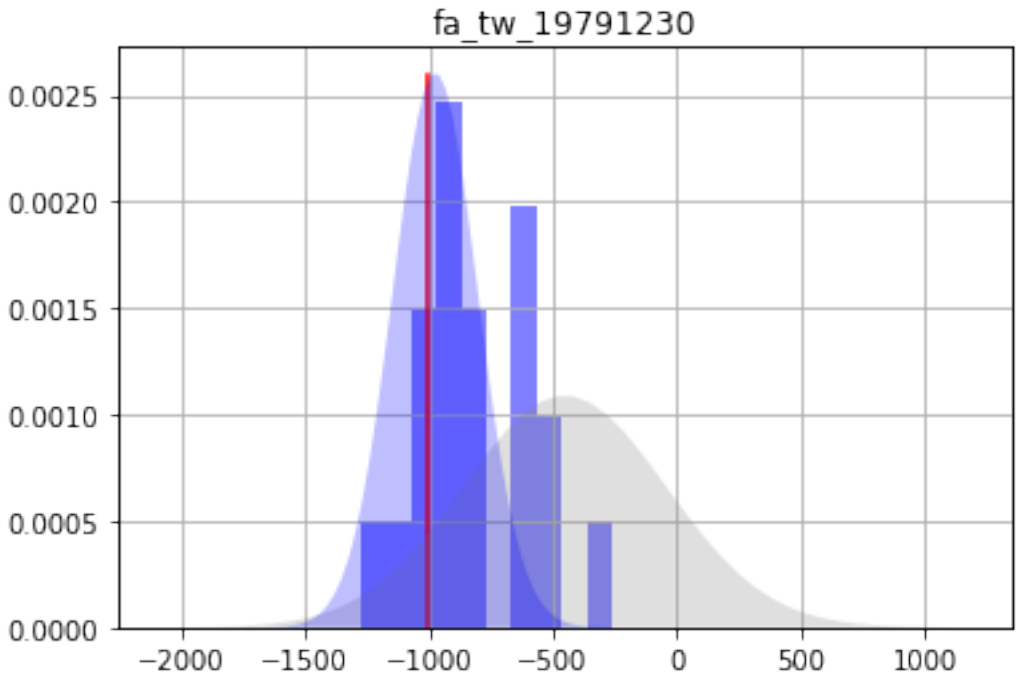
name	prior_mean	prior_stdev	prior_lower_bound	prior_upper_bound	post_mean	post_stdev	post_lower_bound	post_upper_bound
fa_hw_19791230	-977.2390	295.32800	-1567.8900	-386.5840	-1476.8300	247.947000	-1972.7200	-980.9330
fa_hw_19801229	-351.2160	409.77000	-1170.7600	468.3240	-543.4840	336.000000	-1215.4800	128.5170
fa_tw_19791230	-453.0330	409.35100	-1271.7400	365.6690	-974.4930	170.979000	-1316.4500	-632.5340
fa_tw_19801229	108.9600	506.73200	-904.5040	1122.4200	19.0994	263.680000	-508.2600	546.4590
hds_00_013_002_000	39.6102	3.96314	31.6840	47.5365	44.5338	0.274003	43.9858	45.0818
hds_00_013_002_001	38.3838	4.05782	30.2681	46.4994	41.0438	0.687955	39.6678	42.4197
part_status	2.0000	0.00000	2.0000	2.0000	2.0000	0.000000	2.0000	2.0000
part_time	907.7020	704.75100	-501.8010	2317.2000	817.9310	601.413000	-384.8940	2020.7600

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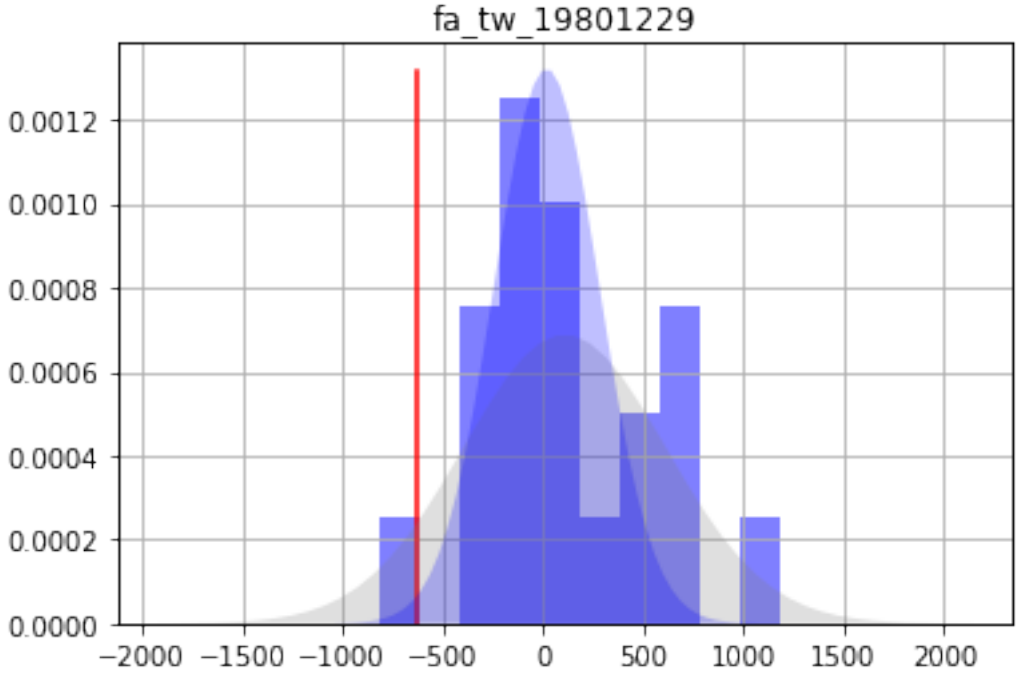
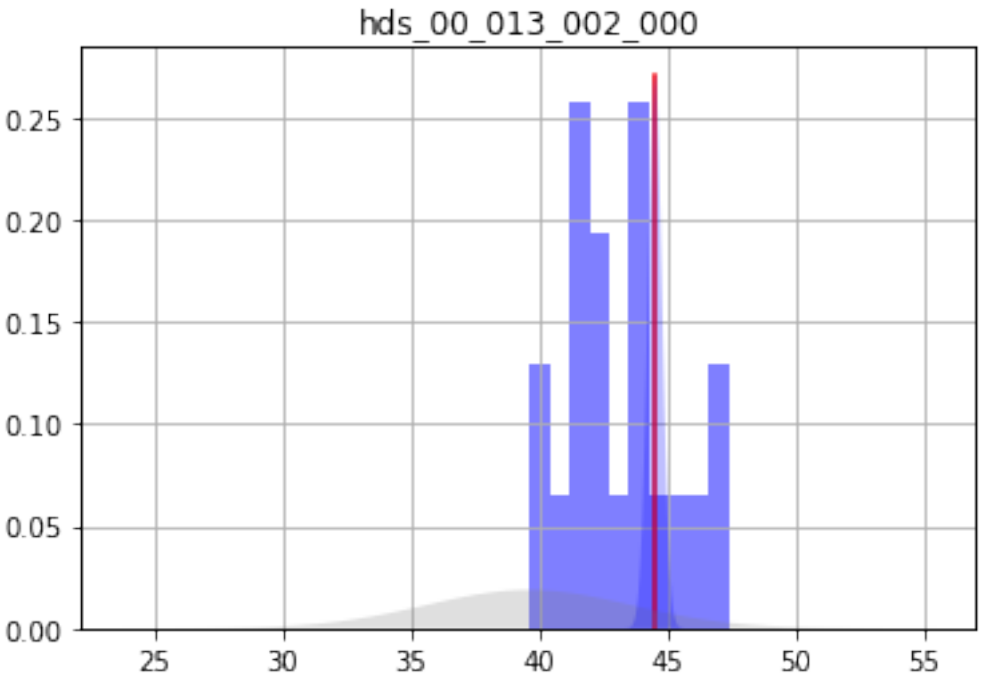
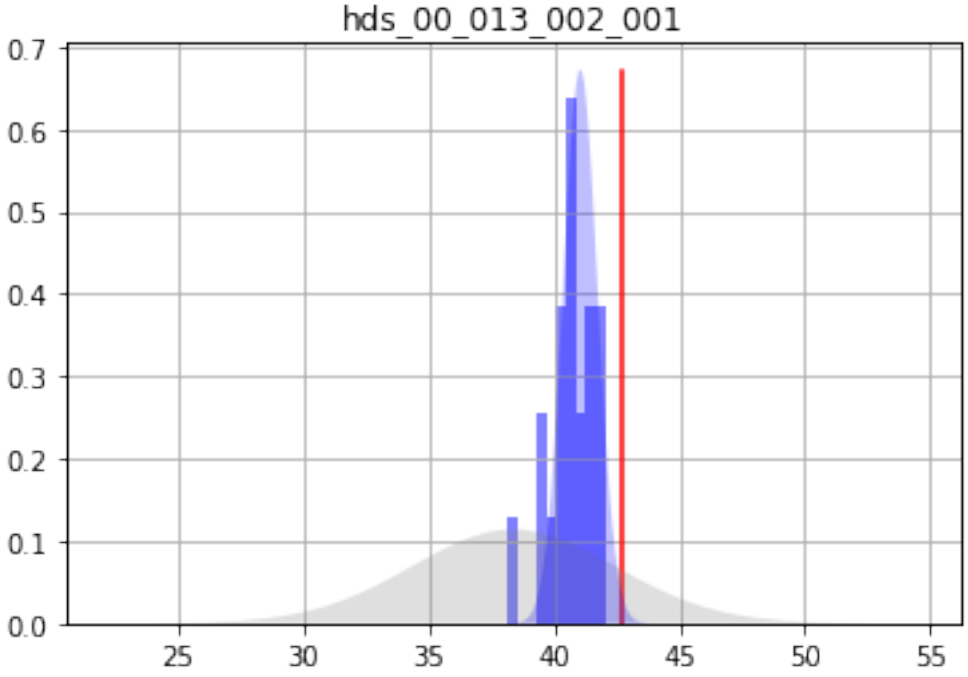
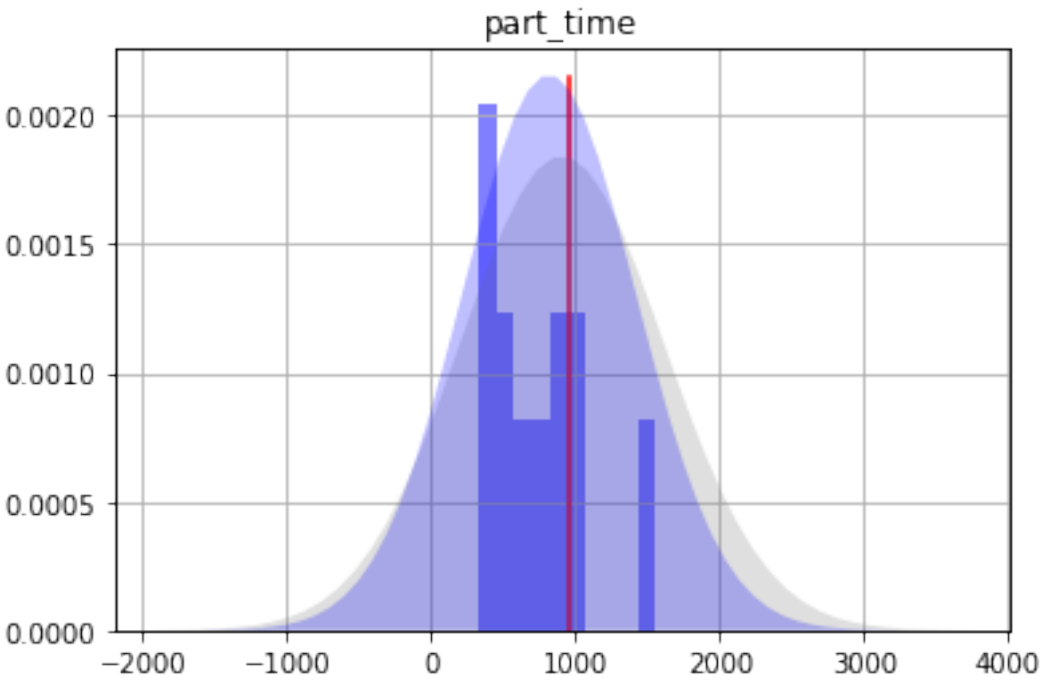
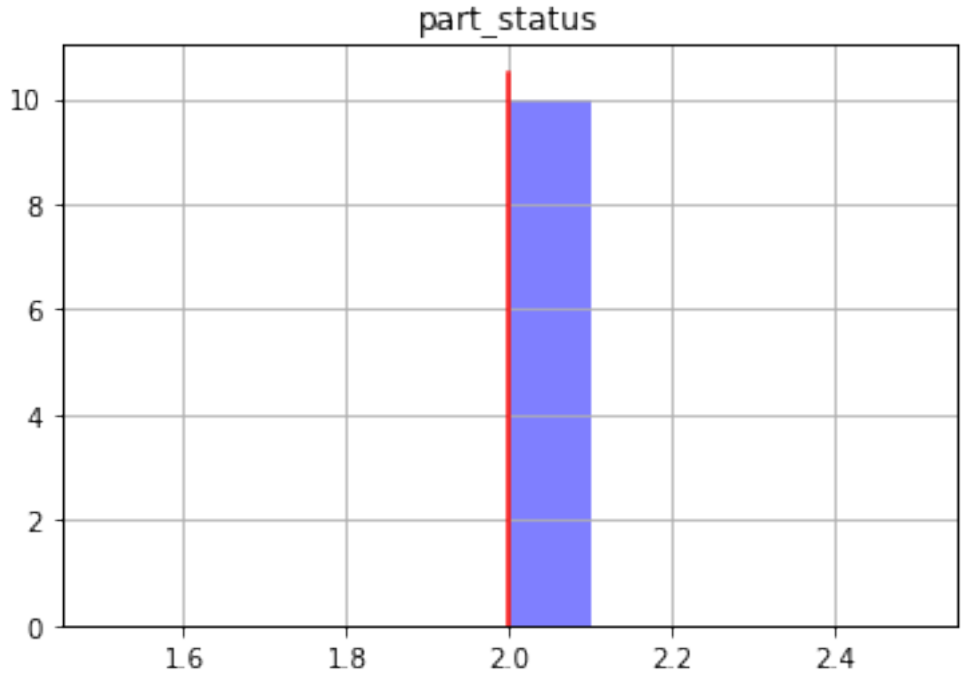
0.0020
0.0015
0.0010
0.0005
0.0000
−2000
−1500
−1000
−500
0
500
1000


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
0.25
0.20
0.15
0.10
0.05
0.00
25
30
35
40
45
50
55


hds_00_013_002_001
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
0.0020
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