pestpp-ies

May 3, 2019

1 Run PESTPP-IES

```
In [1]: import os
        import shutil
        import numpy as np
        import pandas as pd
        import matplotlib.pyplot as plt
        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_ies"
In [3]: pst = pyemu.Pst(os.path.join(t_d, "freyberg.pst"))
        pst.write_par_summary_table(filename="none")
Out[3]:
                                                         initial value \
                             type transform count
                           cn_hk8
                                                  1
                                                                      0
        cn_hk8
                                        log
        gr_prsity4
                      gr_prsity4
                                        log
                                                705
                                                                      0
                                                         0 to 0.176091
                          welflux
                                                  2
        welflux
                                        log
        pp_prsity2
                      pp_prsity2
                                        log
                                                 32
                                                                      0
                          gr_vka4
                                              705
                                                                      0
        gr_vka4
                                        log
                                                                      0
        pp_hk2
                           pp_hk2
                                                 32
                                        log
                                                  1
                                                                      0
        cn_strt7
                         cn_strt7
                                        log
                                                                      0
                                        log
                                                 32
        pp_vka0
                          pp_vka0
        gr_hk4
                                        log
                                                705
                                                                      0
                           gr_hk4
                                                                      0
                                                705
        gr_strt5
                         gr_strt5
                                        log
                                                                      0
        cn_sy6
                           cn_sy6
                                        log
                                                  1
        cn_ss6
                           cn_ss6
                                        log
                                                  1
                                                                      0
                                                                      0
        pp_hk1
                           pp_hk1
                                        log
                                                 32
                         gr_rech2
                                                705
                                                                      0
        gr_rech2
                                        log
                                                705
                                                                      0
        gr_hk3
                           gr_hk3
                                        log
                         gr_strt4
                                                705
                                                                      0
        gr_strt4
                                        log
        cn_strt8
                         cn_strt8
                                        log
                                                  1
                                                                      0
```

| pp_prsity0 | pp_prsity0 | log | 32 | | 0 |
|-------------|---------------------|-------|-------|-------|--------------------|
| cn_prsity6 | cn_prsity6 | log | 1 | | 0 |
| cn_vka6 | cn_vka6 | log | 1 | | 0 |
| pp_sy1 | pp_sy1 | log | 32 | | 0 |
| pp_strt2 | pp_strt2 | log | 32 | | 0 |
| cn_vka7 | cn_vka7 | log | 1 | | 0 |
| gr_sy3 | gr_sy3 | log | 705 | | 0 |
| pp_rech1 | pp_rech1 | log | 32 | | 0 |
| cn_sy8 | cn_sy8 | log | 1 | | 0 |
| gr_sy4 | gr_sy4 | log | 705 | | 0 |
| gr_ss3 | gr_ss3 | log | 705 | | 0 |
| pp_ss0 | pp_ss0 | log | 32 | | 0 |
| pp_ss2 | pp_ss2 | log | 32 | | 0 |
| | | | | | |
| gr_vka3 | gr_vka3 | log | 705 | | 0 |
| gr_ss5 | ${\tt gr_ss5}$ | log | 705 | | 0 |
| gr_ss4 | ${\tt gr_ss4}$ | log | 705 | | 0 |
| cn_vka8 | cn_vka8 | log | 1 | | 0 |
| pp_ss1 | pp_ss1 | log | 32 | | 0 |
| gr_prsity3 | gr_prsity3 | log | 705 | | 0 |
| pp_vka2 | pp_vka2 | log | 32 | | 0 |
| strk | strk | log | 40 | | 0 |
| cn_hk7 | cn_hk7 | log | 1 | | 0 |
| gr_vka5 | gr_vka5 | log | 705 | | 0 |
| flow | flow | log | 1 | | 0 |
| gr_sy5 | gr_sy5 | log | 705 | | 0 |
| pp_vka1 | pp_vka1 | log | 32 | | 0 |
| pp_prsity1 | pp_prsity1 | log | 32 | | 0 |
| gr_strt3 | gr_strt3 | log | 705 | | 0 |
| pp_sy0 | pp_sy0 | log | 32 | | 0 |
| gr_hk5 | gr_hk5 | log | 705 | | 0 |
| cn_ss7 | cn_ss7 | log | 1 | | 0 |
| pp_rech0 | pp_rech0 | log | 32 | | 0 |
| cn_rech4 | cn_rech4 | log | 1 | | 0 |
| gr_prsity5 | | log | 705 | | 0 |
| pp_sy2 | pp_sy2 | log | 32 | | 0 |
| welflux_k02 | | log | 6 | | 0 |
| cn_sy7 | cn_sy7 | log | 1 | | 0 |
| pp_strt1 | pp_strt1 | log | 32 | | 0 |
| cn_ss8 | cn_ss8 | log | 1 | | 0 |
| cn_strt6 | cn_strt6 | log | 1 | | 0 |
| cn_hk6 | cn_hk6 | log | 1 | | 0 |
| cn_prsity7 | ${\tt cn_prsity7}$ | log | 1 | | 0 |
| pp_hk0 | pp_hk0 | log | 32 | | 0 |
| | | h | 7 | . 1 1 | |
| 1-1-0 | upper | bound | Lower | bound | standard deviation |
| cn_hk8 | | 1 | | -1 | 0.5 |
| gr_prsity4 | | 0 | | -1 | 0.25 |

| welflux | 0.176091 to 0.30103 | -0.30103 to 0 | 0.0752575 to 0.11928 |
|------------|---------------------|---------------|----------------------|
| pp_prsity2 | 0 | -1 | 0.25 |
| gr_vka4 | 1 | -1 | 0.5 |
| pp_hk2 | 1 | -1 | 0.5 |
| cn_strt7 | 0.0211893 | -0.0222764 | 0.0108664 |
| pp_vka0 | 1 | -1 | 0.5 |
| gr_hk4 | 1 | -1 | 0.5 |
| gr_strt5 | 0.0211893 | -0.0222764 | 0.0108664 |
| cn_sy6 | 0.243038 | -0.60206 | 0.211275 |
| cn_ss6 | 1 | -1 | 0.5 |
| pp_hk1 | 1 | -1 | 0.5 |
| gr_rech2 | 0.0413927 | -0.0457575 | 0.0217875 |
| gr_hk3 | 1 | -1 | 0.5 |
| gr_strt4 | 0.0211893 | -0.0222764 | 0.0108664 |
| cn_strt8 | 0.0211893 | -0.0222764 | 0.0108664 |
| pp_prsity0 | 0 | -1 | 0.25 |
| cn_prsity6 | 0 | -1 | 0.25 |
| cn_vka6 | 1 | -1 | 0.5 |
| pp_sy1 | 0.243038 | -0.60206 | 0.211275 |
| pp_strt2 | 0.0211893 | -0.0222764 | 0.0108664 |
| cn_vka7 | 1 | -1 | 0.5 |
| gr_sy3 | 0.243038 | -0.60206 | 0.211275 |
| pp_rech1 | 0.0413927 | -0.0457575 | 0.0217875 |
| cn_sy8 | 0.243038 | -0.60206 | 0.211275 |
| gr_sy4 | 0.243038 | -0.60206 | 0.211275 |
| gr_ss3 | 1 | -1 | 0.5 |
| pp_ss0 | 1 | -1 | 0.5 |
| pp_ss2 | 1 | -1 | 0.5 |
| | • • • | | • • • |
| gr_vka3 | 1 | -1 | 0.5 |
| gr_ss5 | 1 | -1 | 0.5 |
| gr_ss4 | 1 | -1 | 0.5 |
| cn_vka8 | 1 | -1 | 0.5 |
| pp_ss1 | 1 | -1 | 0.5 |
| gr_prsity3 | 0 | -1 | 0.25 |
| pp_vka2 | 1 | -1 | 0.5 |
| strk | 2 | -2 | 1 |
| cn_hk7 | 1 | -1 | 0.5 |
| gr_vka5 | 1 | -1 | 0.5 |
| flow | 0.09691 | -0.124939 | 0.0554622 |
| gr_sy5 | 0.243038 | -0.60206 | 0.211275 |
| pp_vka1 | 1 | -1 | 0.5 |
| pp_prsity1 | 0 | -1 | 0.25 |
| gr_strt3 | 0.0211893 | -0.0222764 | 0.0108664 |
| pp_sy0 | 0.243038 | -0.60206 | 0.211275 |
| gr_hk5 | 1 | -1 | 0.5 |
| cn_ss7 | 1 | -1 | 0.5 |
| pp_rech0 | 0.0413927 | -0.0457575 | 0.0217875 |

```
cn_rech4
                        0.0791812
                                             -0.09691
                                                                  0.0440228
                                                                        0.25
gr_prsity5
                                                   -1
                         0.243038
                                             -0.60206
                                                                    0.211275
pp_sy2
welflux_k02
                                1
                                                                         0.5
                         0.243038
                                            -0.60206
                                                                   0.211275
cn_sy7
pp_strt1
                        0.0211893
                                           -0.0222764
                                                                  0.0108664
cn_ss8
                                                                         0.5
                        0.0211893
                                           -0.0222764
                                                                  0.0108664
cn_strt6
cn hk6
                                                                         0.5
                                0
                                                   -1
                                                                        0.25
cn_prsity7
pp_hk0
                                1
                                                   -1
                                                                         0.5
```

[65 rows x 7 columns]

Should we fix either PP or grids?

plt.show()

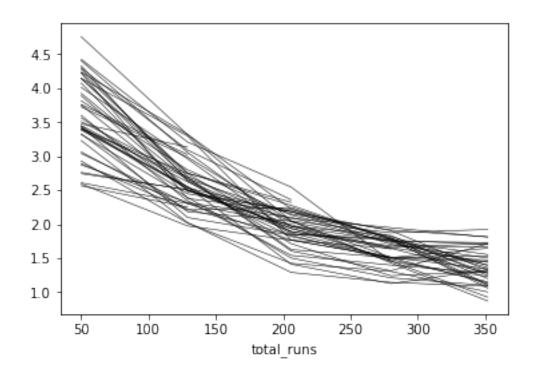
phi.iloc[-1,6:].hist()

```
In [4]: par = pst.parameter_data
    # grid pars
    #should_fix = par.loc[par.pargp.apply(lambda x: "gr" in x), "parnme"]
    # pp pars
    #should_fix = par.loc[par.pargp.apply(lambda x: "pp" in x), "parnme"]

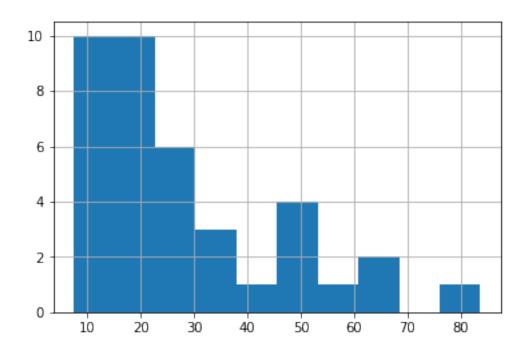
# if we want to fix some pars, do it here
    #pst.parameter_data.loc[should_fix, "partrans"] = "fixed"
    #pst.npar,pst.npar_adj
```

1.0.1 Run PESTPP-IES in original mode and post process

phi.iloc[:,6:].apply(np.log10).plot(legend=False,lw=0.5,color='k')

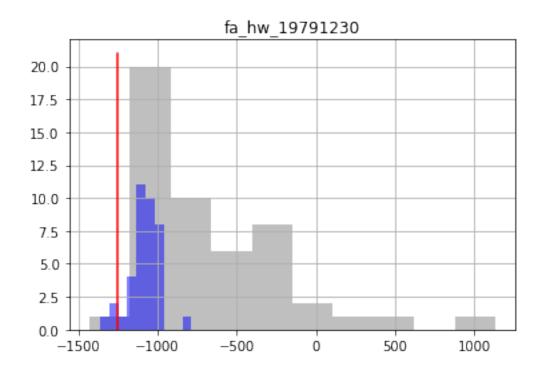


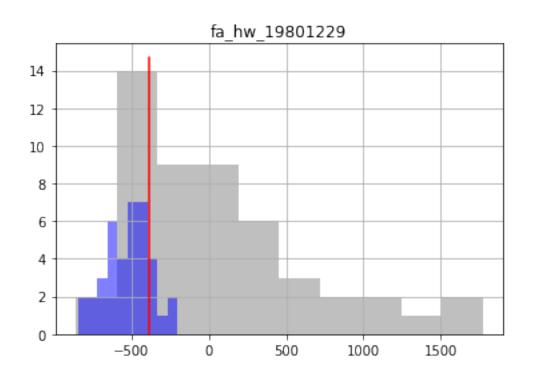
Out[8]: <matplotlib.axes._subplots.AxesSubplot at 0x1823d8db00>

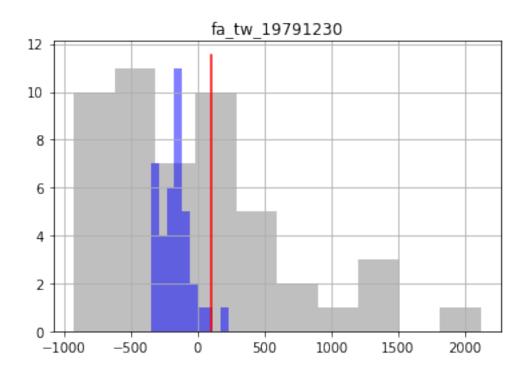


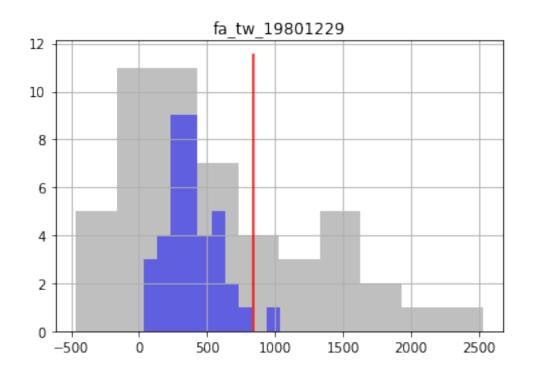
Plot forecast prior and posterior histograms with "truth" (red line)

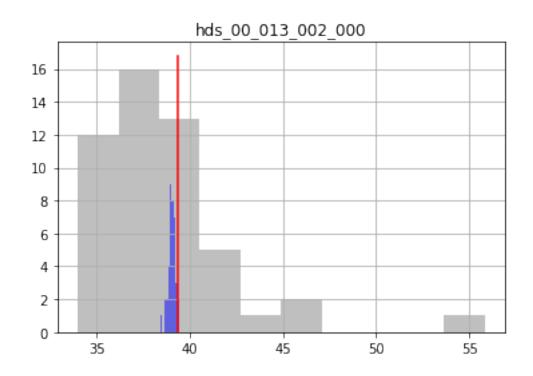
```
In [9]: oe_pr = pd.read_csv(os.path.join(m_d,"freyberg_ies.0.obs.csv"),index_col=0)
    oe_pt = pd.read_csv(os.path.join(m_d,"freyberg_ies.{0}.obs.csv".format(pst.control_data
    obs = pst.observation_data
    fnames = pst.pestpp_options["forecasts"].split(",")
    for forecast in fnames:
        ax = plt.subplot(111)
        oe_pr.loc[:,forecast].hist(ax=ax,color="0.5",alpha=0.5)
        oe_pt.loc[:,forecast].hist(ax=ax,color="b",alpha=0.5)
        ax.plot([obs.loc[forecast,"obsval"],obs.loc[forecast,"obsval"]],ax.get_ylim(),"r")
        ax.set_title(forecast)
        plt.show()
```

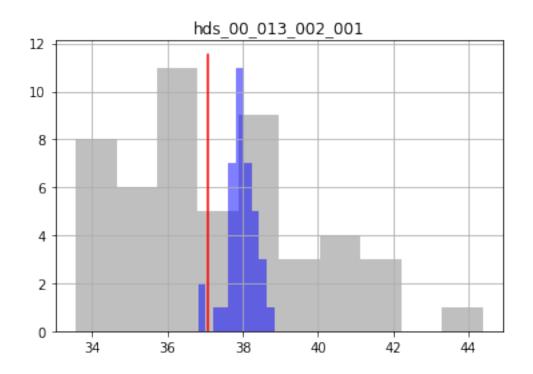


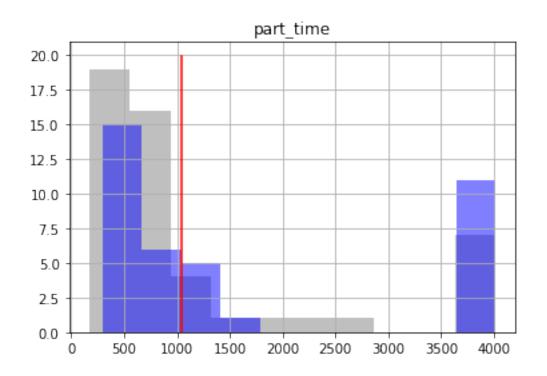


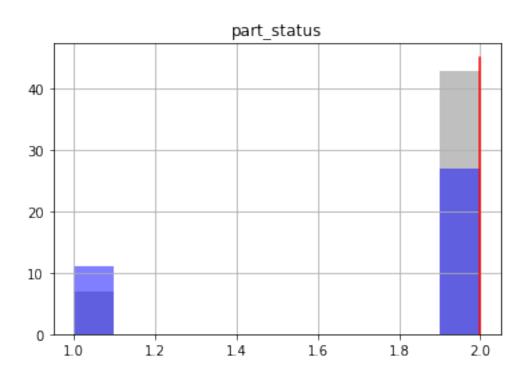




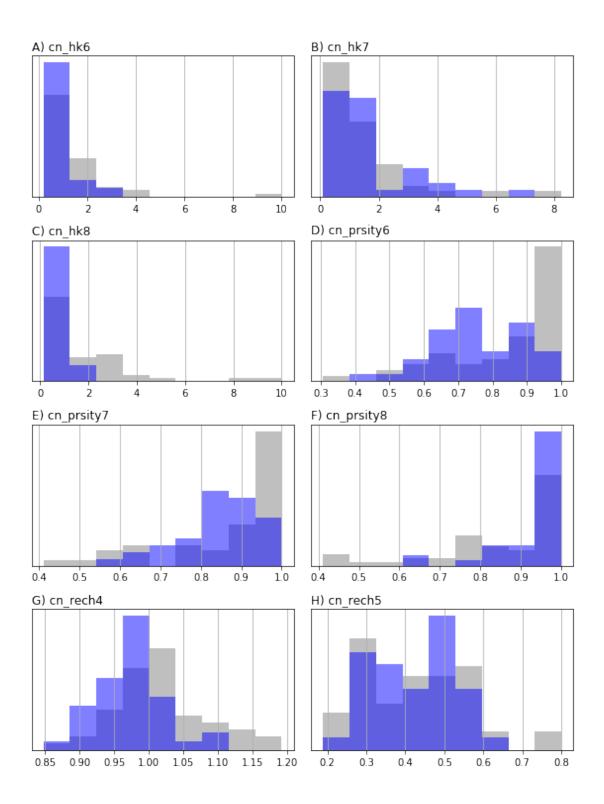


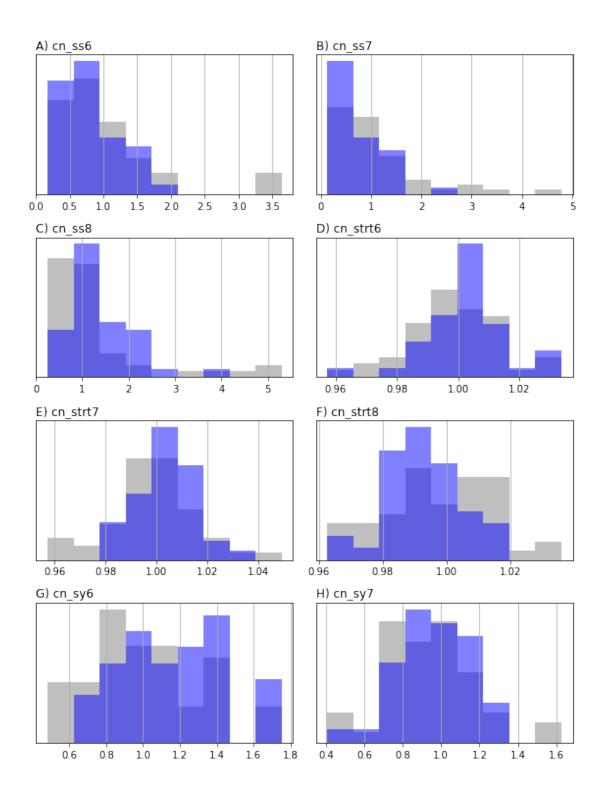


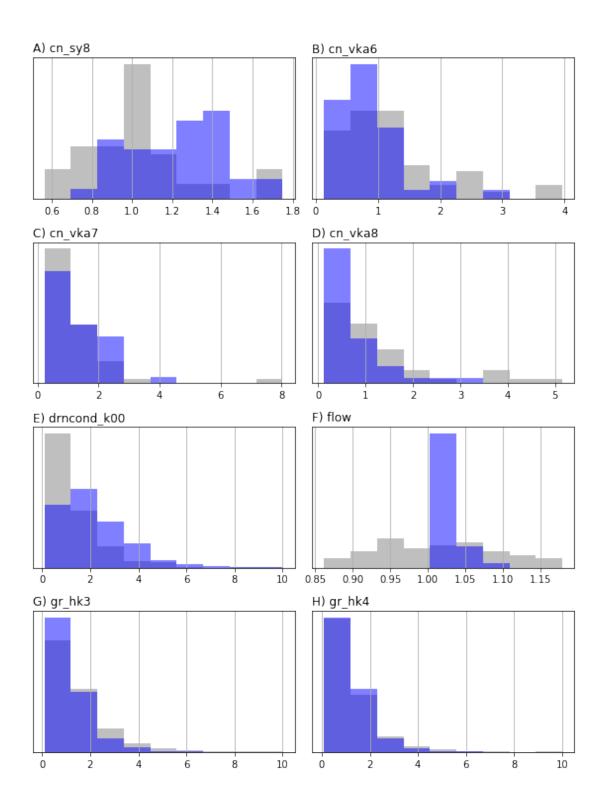


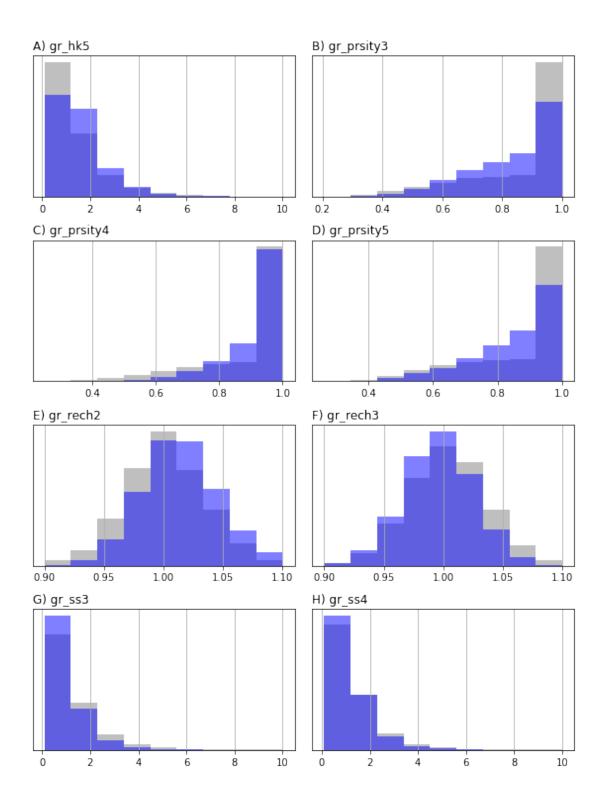


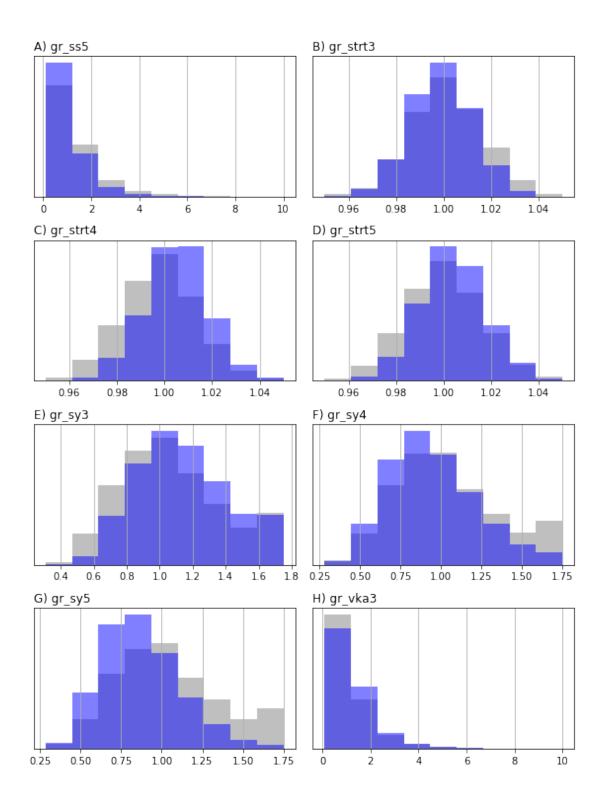
Plot parameter histograms by group

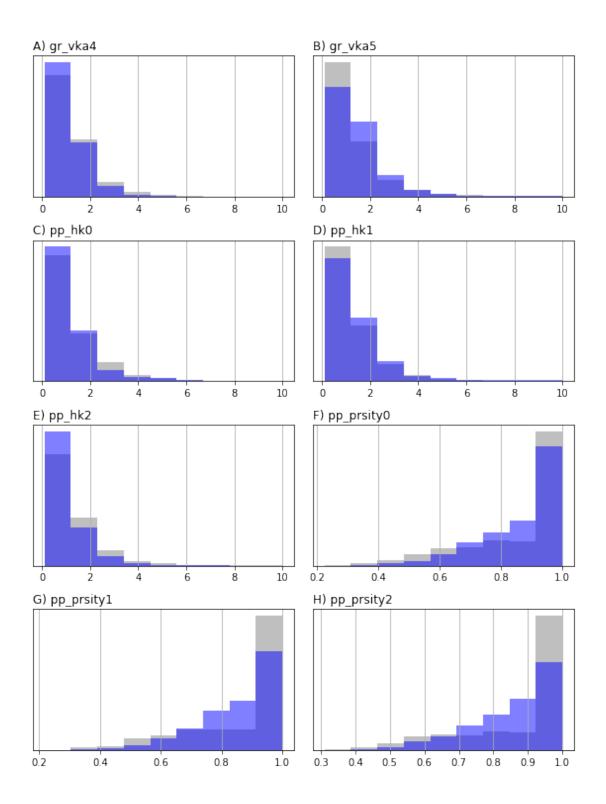


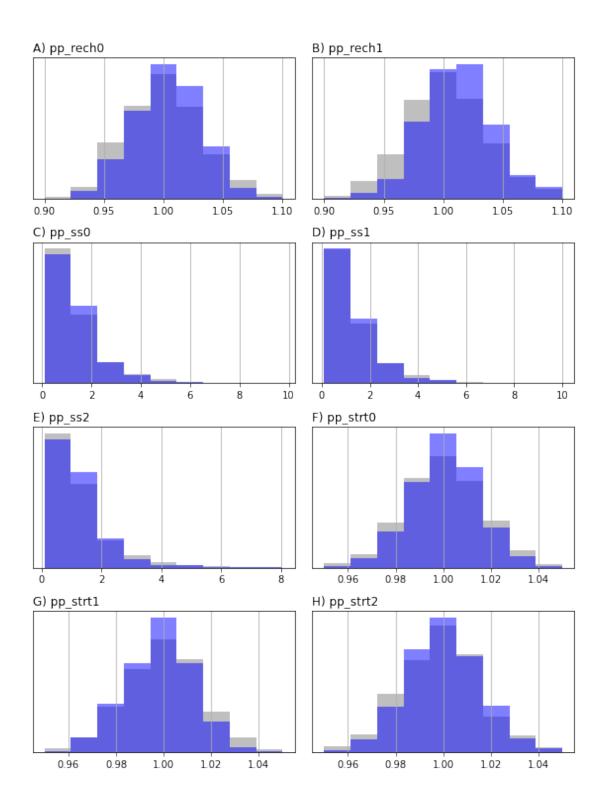


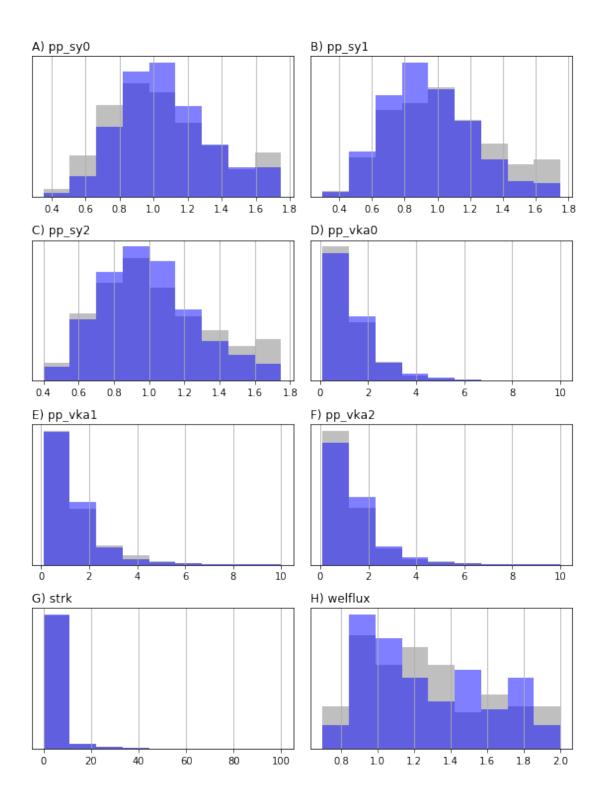












A) welflux_k02

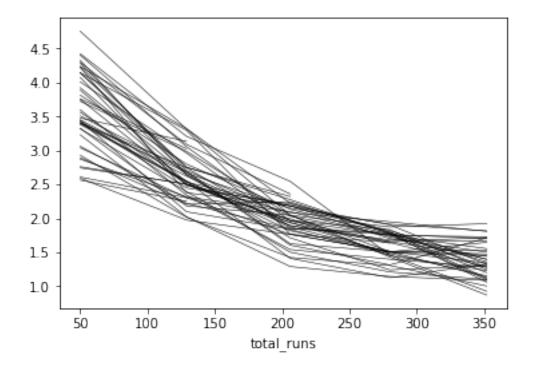
```
# pe_pr.loc[:,li] = pe_pr.loc[:,li].apply(np.log10)
# pe_pr.shape
```

Those are some pretty extreme variance reductions, considering we are conditioning 10K+ pars on 13 water levels and one flux. This is a well-known issue with low-rank ensemble method ("ensemble collapse"). This is over come with localization....

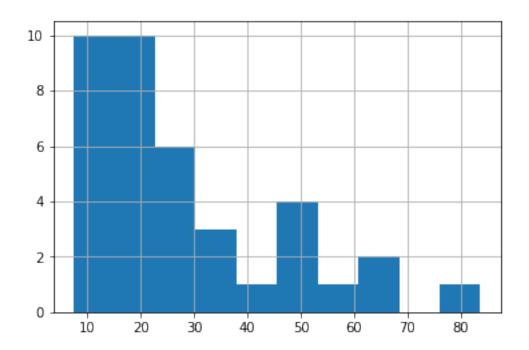
1.0.2 PESTPP-IES with simple temporal localization (and common sense)

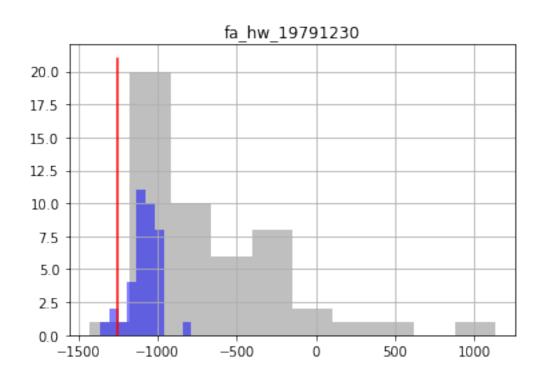
Now let's add some localization. The obvious stuff is temporal - scenario parameters can't influence historic observations (and the inverse is true) so let's tell PESTPP-IES about this. Also, should porosity be adjusted at all given the observations we have???

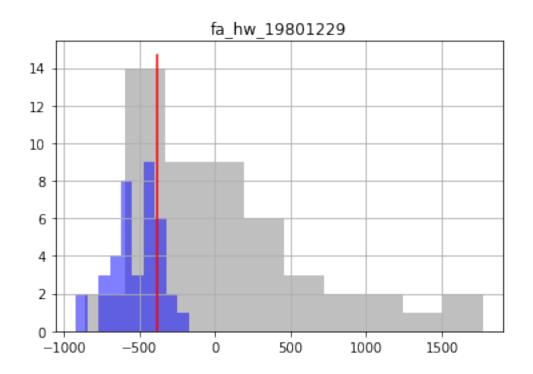
```
In [12]: par = pst.parameter_data
         #parameter groups for future recharge
         dont_groups = [g for g in pst.par_groups if "pr" in g]
         dont_groups.extend(["gr_rech3","pp_rech1","cn_rech5"])
         dont_groups = [g for g in dont_groups if g in pst.adj_par_groups]
         dont_pars = par.loc[par.pargp.apply(lambda x: x in dont_groups),"parnme"].tolist()
         dont_pars.append("welflux_001")
         dont_groups.append("welflux_001")
         dont_groups
Out[12]: ['gr_prsity4',
          'pp_prsity2',
          'pp_prsity0',
          'cn_prsity6',
          'cn_prsity8',
          'gr_prsity3',
          'pp_prsity1',
          'gr_prsity5',
          'cn_prsity7',
          'gr_rech3',
          'pp_rech1',
          'cn_rech5',
          'welflux_001']
In [13]: cols = pst.adj_par_groups
         cols.remove("welflux")
         cols.extend(["welflux_000","welflux_001"])
         loc = pyemu.Matrix.from_names(pst.nnz_obs_names,cols).to_dataframe()
         loc.loc[:,:]= 1.0
         loc.loc[:,dont_groups] = 0.0
         pyemu.Matrix.from_dataframe(loc).to_ascii(os.path.join(t_d,"loc.mat"))
In [14]: pst.pestpp_options["ies_localizer"] = "loc.mat"
         pst.write(os.path.join(t_d,"freyberg_ies.pst"))
         pyemu.os_utils.start_slaves(t_d,"pestpp-ies","freyberg_ies.pst",num_slaves=20,master_e
```

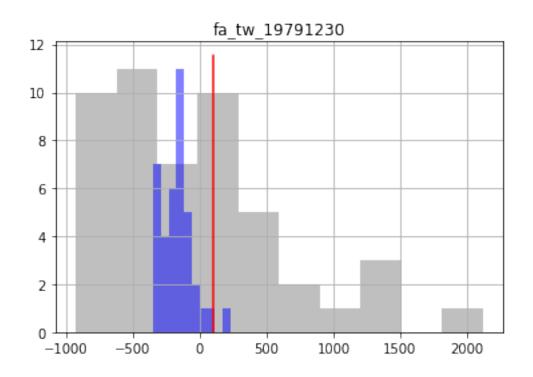


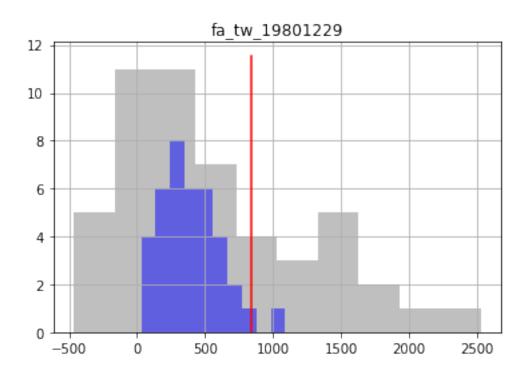
Out[15]: <matplotlib.axes._subplots.AxesSubplot at 0x1828c5bf28>

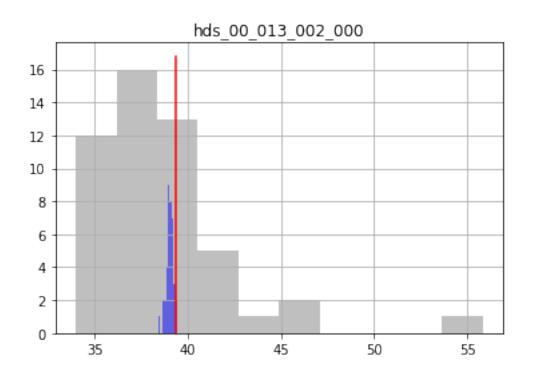


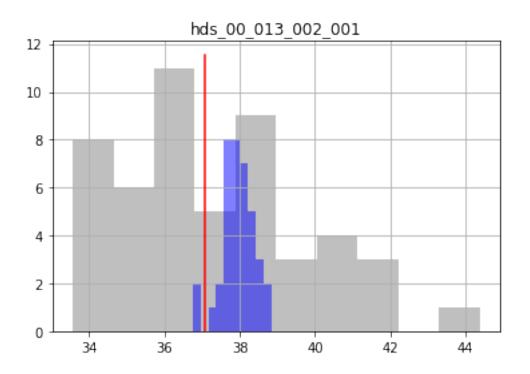


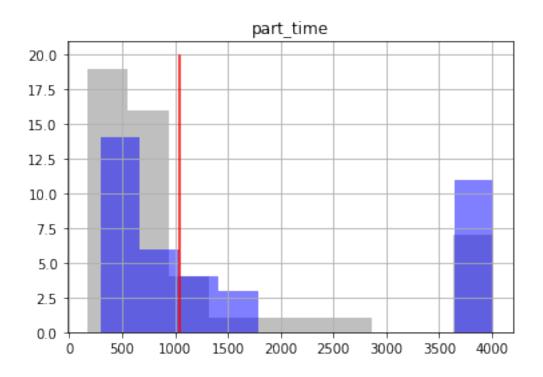


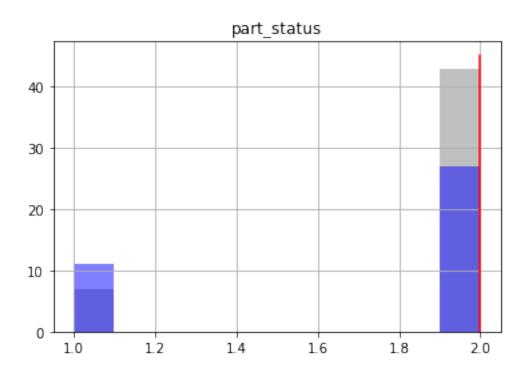








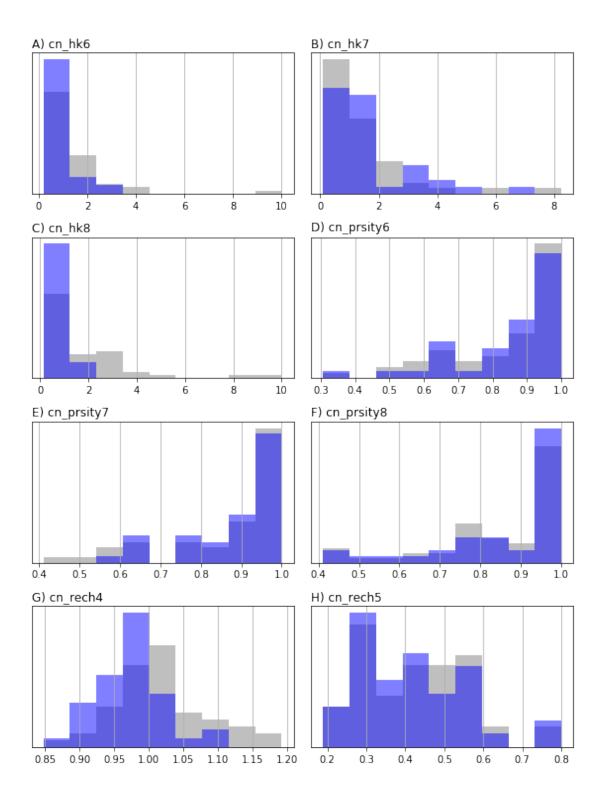


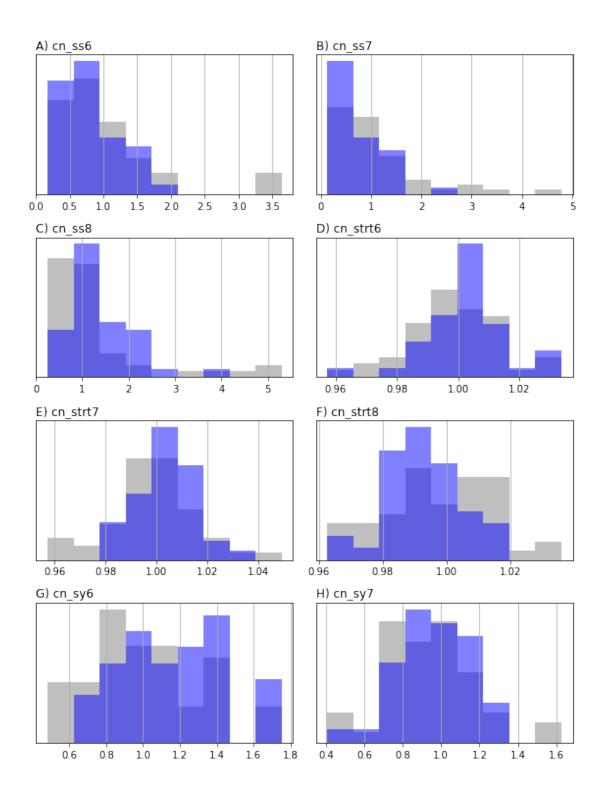


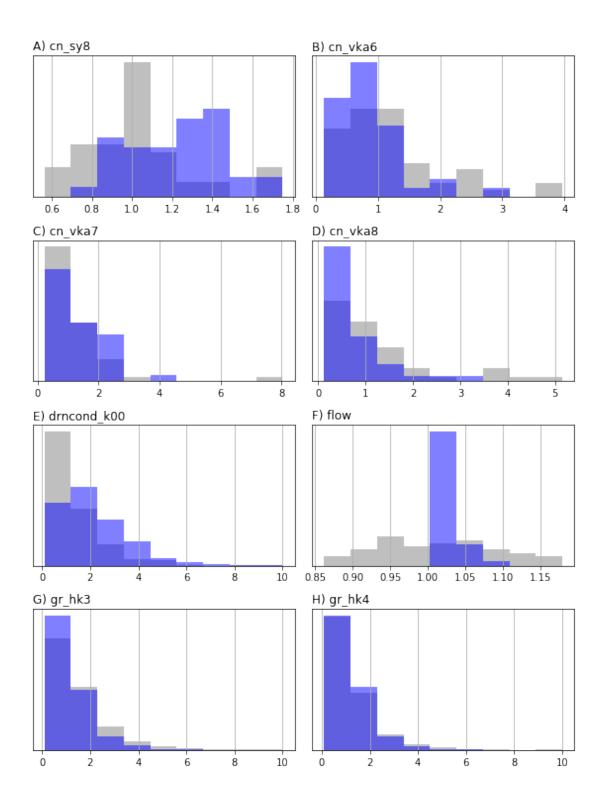
```
#pe_pr.index = pe_pt.index
#par = pst.parameter_data
print(pe_pr.shape,pe_pt.shape)
pdict = par.groupby("pargp").groups
pyemu.plot_utils.ensemble_helper({"0.5":pe_pr,"b":pe_pt},plot_cols=pdict)
#pyemu.plot_utils.ensemble_change_summary(pe_pr,pe_pt,pst=pst,bins=20)

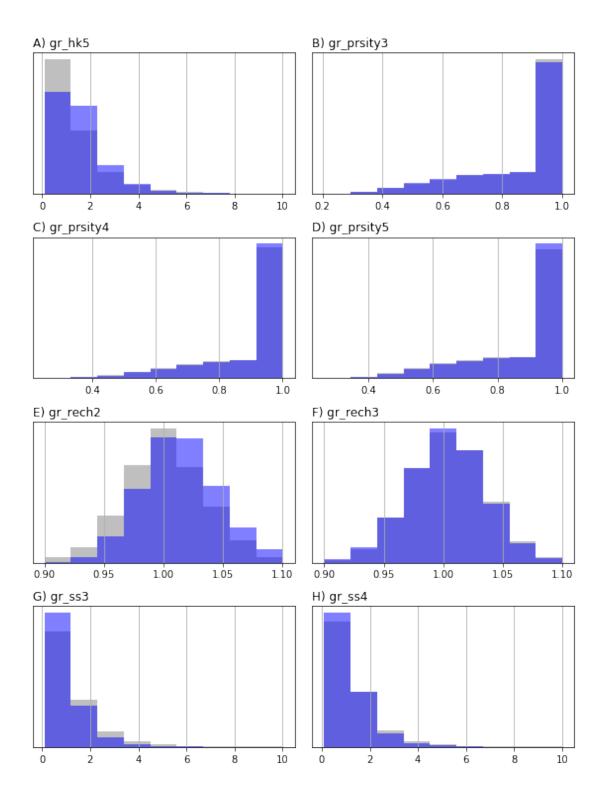
(50, 14819) (38, 14819)

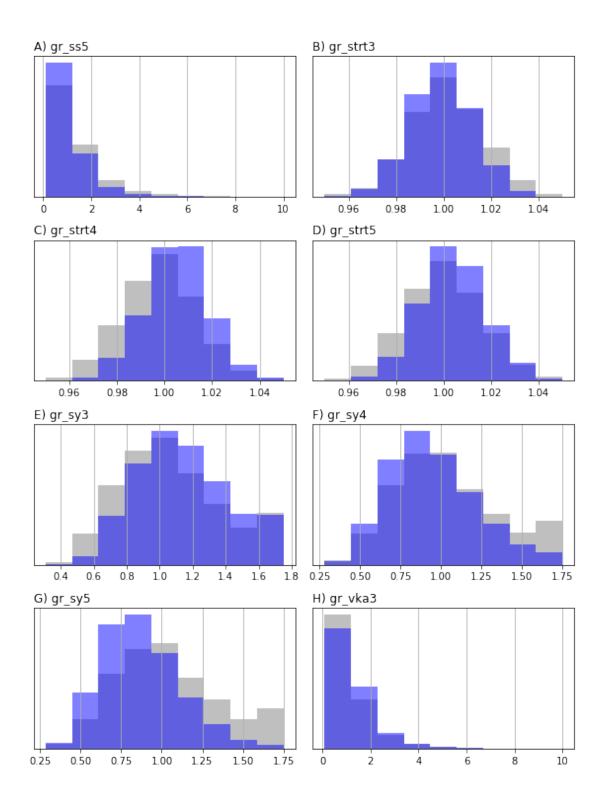
<Figure size 576x756 with 0 Axes>
```

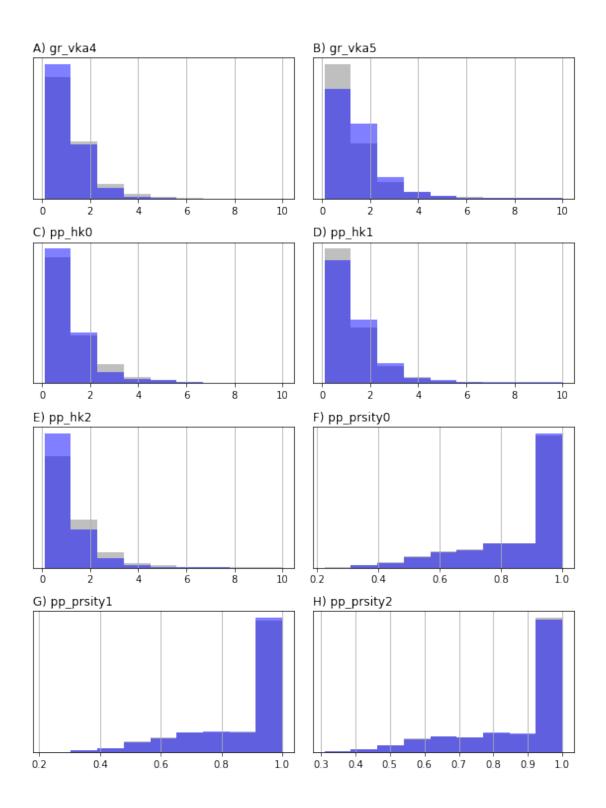


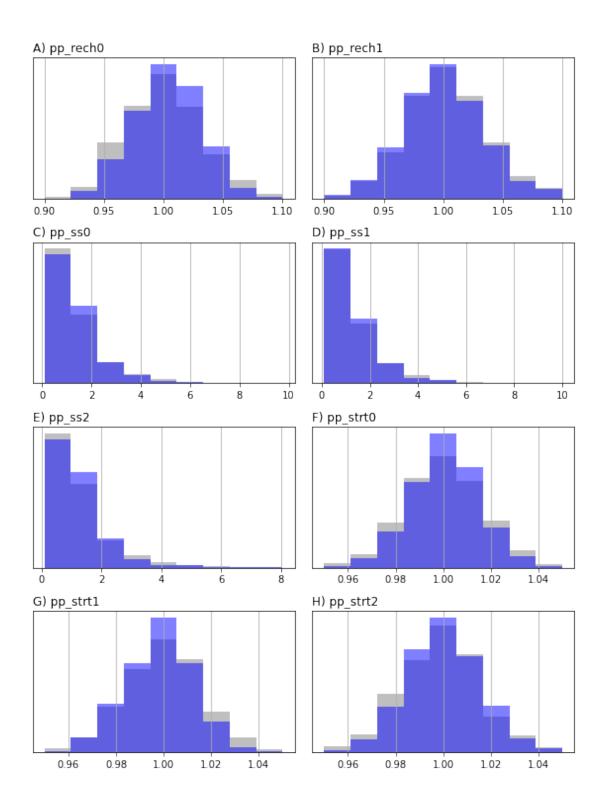


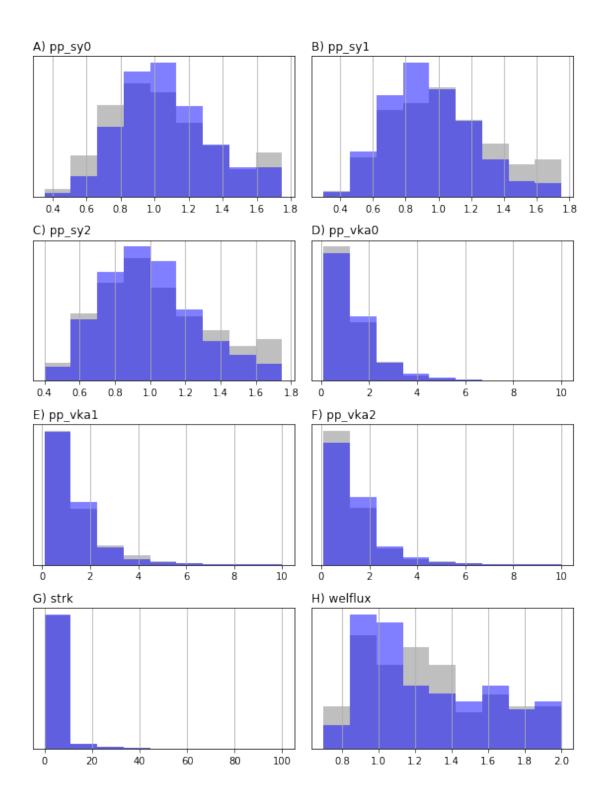


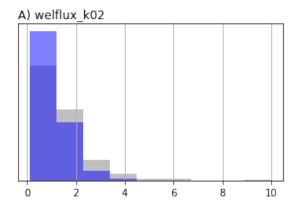










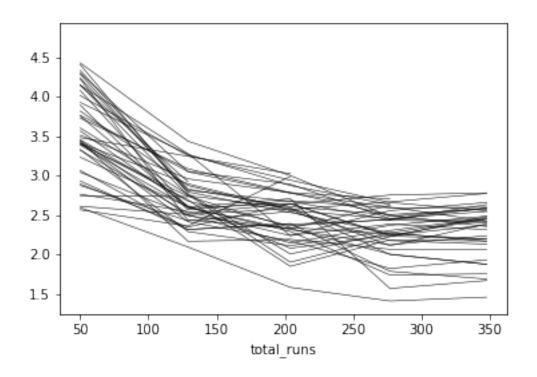


1.0.3 PESTPP-IES with par-by-par distance based localization

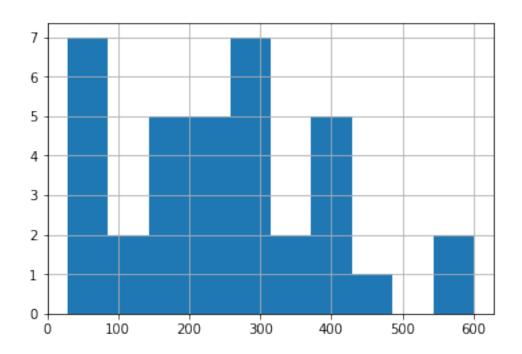
```
In [18]: m = flopy.modflow.Modflow.load("freyberg.nam",model_ws="template")
```

```
In [19]: par = pst.parameter_data
         gr_par = par.loc[par.pargp.apply(lambda x: "gr" in x and "prsity" not in x),:].copy()
         print(gr_par.pargp.unique())
         gr_par.groupby("pargp").groups
         gr_par.loc[:,"i"] = gr_par.parnme.apply(lambda x: int(x[-6:-3]))
         gr_par.loc[:,"j"] = gr_par.parnme.apply(lambda x: int(x[-3:]))
         gr_par.loc[:,"x"] = gr_par.apply(lambda x: m.sr.xcentergrid[x.i,x.j],axis=1)
         gr_par.loc[:,"y"] = gr_par.apply(lambda x: m.sr.ycentergrid[x.i,x.j],axis=1)
         obs = pst.observation_data
         nobs = obs.loc[obs.obgnme=="calhead",:].copy()
         nobs.loc[:,"i"] = nobs.obsnme.apply(lambda x: int(x.split('_')[2]))
         nobs.loc[:,"j"] = nobs.obsnme.apply(lambda x: int(x.split('_')[3]))
         nobs.loc[:,"x"] = nobs.apply(lambda x: m.sr.xcentergrid[x.i,x.j],axis=1)
         nobs.loc[:,"y"] = nobs.apply(lambda x: m.sr.ycentergrid[x.i,x.j],axis=1)
         pp_tpl = [f for f in os.listdir(t_d) if "pp" in f and f.endswith(".tpl")]
         pp_tpl_dfs = [pyemu.pp_utils.pp_tpl_to_dataframe(os.path.join(t_d,f)) for f in pp_tpl_
         pp_par = pd.concat(pp_tpl_dfs)
         pp_par.index = pp_par.parnme
         \#pp\_par = par.loc[par.pargp.apply(lambda x: "pp" in x),:].copy()
['gr_hk3' 'gr_hk4' 'gr_hk5' 'gr_rech2' 'gr_rech3' 'gr_ss3' 'gr_ss4'
 'gr_ss5' 'gr_strt3' 'gr_strt4' 'gr_strt5' 'gr_sy3' 'gr_sy4' 'gr_sy5'
 'gr_vka3' 'gr_vka4' 'gr_vka5']
In [20]: loc = pyemu.Matrix.from_names(pst.nnz_obs_names,pst.adj_par_names).to_dataframe()
         loc.loc[:,:] = 1.0
         loc_dist = 5000.0
         sadj = set(pst.adj_par_names)
         for oname in obs.loc[obs.obgnme=="calhead","obsnme"]:
             xx,yy = nobs.loc[oname,['x','y']]
             gr_par.loc[:,"dist"] = gr_par.apply(lambda x: (x.x - xx)**2 + (x.y - yy)**2,axis=
             gr_too_far = gr_par.loc[gr_par.dist > loc_dist,"parnme"]
             gr_too_far = gr_too_far.loc[gr_too_far.apply(lambda x: x in sadj)]
             loc.loc[:,gr_too_far] = 0.0
             pp_par.loc[:,"dist"] = pp_par.apply(lambda x: (x.x - xx)**2 + (x.y - yy)**2,axis=
             pp_too_far = pp_par.loc[pp_par.dist > loc_dist,"parnme"]
             pp_too_far = pp_too_far.loc[pp_too_far.apply(lambda x: x in sadj)]
             loc.loc[oname,pp_too_far] = 0.0
             print(oname,gr_too_far.shape[0]/gr_par.shape[0],pp_too_far.shape[0]/pp_par.shape[0]
         loc.loc[:,dont_pars] = 0.0
```

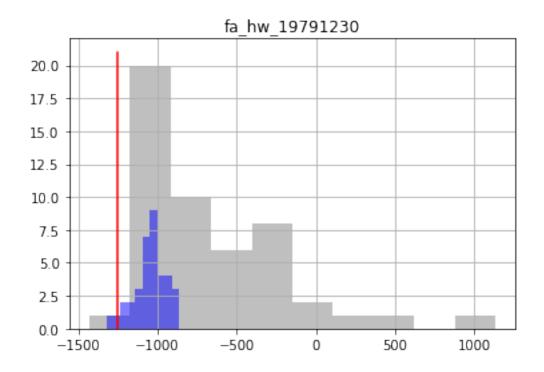
```
\#spars = par.loc[par.parnme.apply(lambda <math>x: "ss" in x or "sy" in x), "parnme"]
         \#loc.loc[:,spars] = 0.0
         loc.sum(axis=1)
hds_00_002_009_000 0.46382978723404256 0.46875
hds_00_002_015_000 0.4794326241134752 0.5
hds_00_003_008_000 0.43829787234042555 0.34375
hds_00_009_001_000 0.3304964539007092 0.25
hds_00_013_010_000 0.15319148936170213 0.09375
hds_00_015_016_000 0.13900709219858157 0.0625
hds_00_021_010_000 0.06950354609929078 0.03125
hds_00_022_015_000 0.12198581560283688 0.15625
hds_00_024_004_000 0.17872340425531916 0.15625
hds_00_026_006_000 0.2198581560283688 0.21875
hds_00_029_015_000 0.29929078014184396 0.28125
hds_00_033_007_000 0.3829787234042553 0.375
hds_00_034_010_000 0.4 0.40625
Out[20]: fo_39_19791230
                               1786.0
         hds_00_002_009_000
                               1546.0
         hds_00_002_015_000
                               1530.0
         hds_00_003_008_000
                               1610.0
         hds_00_009_001_000
                               1658.0
         hds_00_013_010_000
                               1738.0
         hds_00_015_016_000
                               1754.0
         hds_00_021_010_000
                               1770.0
         hds_00_022_015_000
                               1706.0
         hds_00_024_004_000
                               1706.0
         hds_00_026_006_000
                               1674.0
         hds_00_029_015_000
                               1642.0
         hds_00_033_007_000
                               1594.0
         hds_00_034_010_000
                               1578.0
         dtype: float64
In [21]: pyemu.Matrix.from_dataframe(loc).to_coo(os.path.join(t_d,"loc.jcb"))
         pst.pestpp_options["ies_localizer"] = "loc.jcb"
         pst.write(os.path.join(t_d,"freyberg_ies.pst"))
In [22]: pyemu.os_utils.start_slaves(t_d, "pestpp-ies", "freyberg_ies.pst", num_slaves=20, master_
In [23]: phi = pd.read_csv(os.path.join(m_d, "freyberg_ies.phi.actual.csv"), index_col=0)
         phi.index = phi.total_runs
         phi.iloc[:,6:].apply(np.log10).plot(legend=False,lw=0.5,color='k')
         plt.show()
         phi.iloc[-1,6:].hist()
```

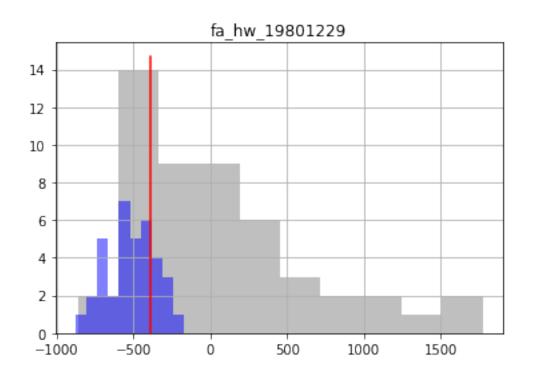


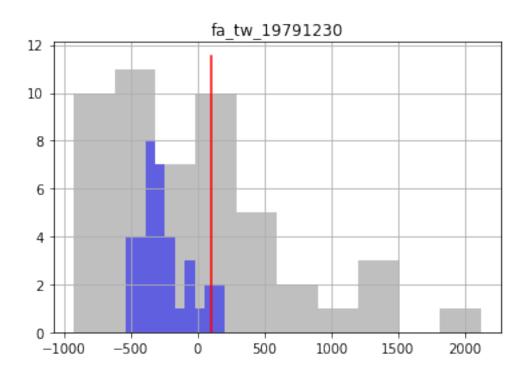
Out[23]: <matplotlib.axes._subplots.AxesSubplot at 0x18269910b8>

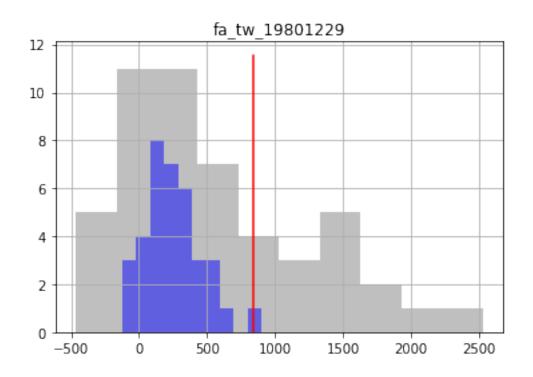


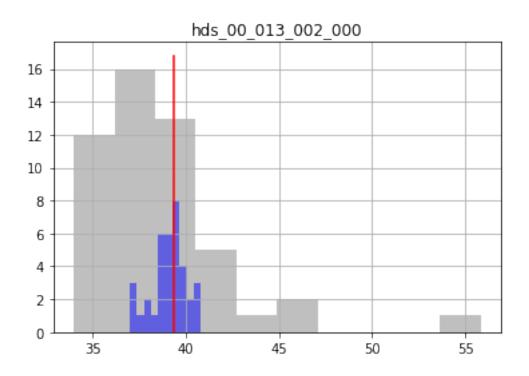
```
In [24]: oe_pr = pd.read_csv(os.path.join(m_d, "freyberg_ies.0.obs.csv"),index_col=0)
    oe_pt = pd.read_csv(os.path.join(m_d, "freyberg_ies.{0}.obs.csv".format(pst.control_data)
    obs = pst.observation_data
    fnames = pst.pestpp_options["forecasts"].split(",")
    for forecast in fnames:
        ax = plt.subplot(111)
        oe_pr.loc[:,forecast].hist(ax=ax,color="0.5",alpha=0.5)
        oe_pt.loc[:,forecast].hist(ax=ax,color="b",alpha=0.5)
        ax.plot([obs.loc[forecast,"obsval"],obs.loc[forecast,"obsval"]],ax.get_ylim(),"r".ax.set_title(forecast)
        plt.show()
```

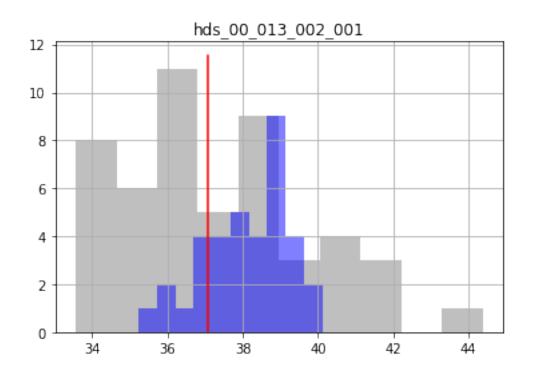


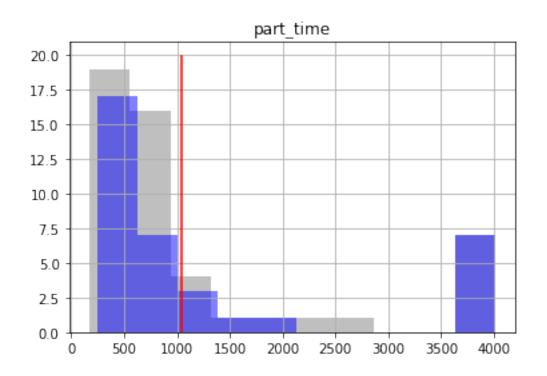


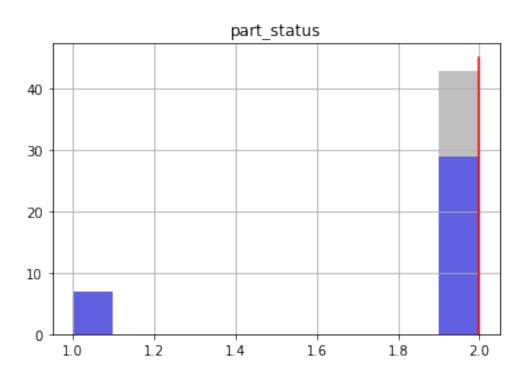












<Figure size 576x756 with 0 Axes>

