# pestpp-ies

May 18, 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 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_ies"
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 upper bound \
                       gr_strt3
                                             705
                                                                0.0211893
       gr_strt3
                                      log
                                             705
                                                             0
                                                                 0.243038
       gr_sy5
                         gr_sy5
                                      log
                                             32
                                                             0 0.0211893
                                      log
       pp_strt0
                       pp_strt0
                                              32
                                                             0
       pp_hk2
                        pp_hk2
                                      log
                                                             0
                                                                 0.176091
        cn_prsity6
                     cn_prsity6
                                      log
                                              1
                                                                 0.243038
                                                             0
       cn_sy7
                         cn_sy7
                                      log
                                               1
                                      log
                                             705
                                                             0
       gr_ss4
                         gr_ss4
                         pp_sy0
                                             32
                                                             0 0.243038
       pp_sy0
                                      log
                       gr_rech2
                                           705
                                                             0
                                                               0.0413927
       gr_rech2
                                      log
       strk
                           strk
                                      log
                                              40
                                                             0
                      cn_strt8
                                      log
                                              1
                                                             0
                                                                0.0211893
       cn_strt8
                                              32
                                                                 0.243038
       pp_sy2
                         pp_sy2
                                      log
```

hl-7	hl-7	7	4	0	4
cn_hk7	cn_hk7	log	1	0	1
pp_rech1	pp_rech1	log	32	0	0.0413927
pp_strt2	pp_strt2	log	32	0	0.0211893
cn_vka6	cn_vka6	log	1	0	1
pp_vka1	pp_vka1	log	32	0	1
cn_ss8	cn_ss8	log	1	0	1
cn_rech4	cn_rech4	log	1	0	0.0791812
gr_prsity5	gr_prsity5	log	705	0	0.176091
pp_hk0	pp_hk0	log	32	0	1
cn_ss7	cn_ss7	log	1	0	1
pp_ss2	pp_ss2	log	32	0	1
gr_sy4	gr_sy4	log	705	0	0.243038
cn_prsity7	cn_prsity7	log	1	0	0.176091
gr_prsity3	gr_prsity3	log	705	0	0.176091
cn_vka7	cn_vka7	log	1	0	1
pp_ss1	pp_ss1	log	32	0	1
pp_prsity0	pp_prsity0	log	32	0	0.176091
pp_ss0	pp_ss0	log	32	0	1
gr_prsity4	gr_prsity4	log	705	0	0.176091
gr_ss5	${\tt gr\_ss5}$	log	705	0	1
gr_vka5	gr_vka5	log	705	0	1
pp_vka2	pp_vka2	log	32	0	1
gr_strt5	gr_strt5	log	705	0	0.0211893
cn_sy6	cn_sy6	log	1	0	0.243038
pp_prsity1	pp_prsity1	log	32	0	0.176091
gr_ss3	gr_ss3	log	705	0	1
gr_sy3	gr_sy3	log	705	0	0.243038
cn_hk8	cn_hk8	log	1	0	1
drncond_k00	drncond_k00	log	10	0	1
gr_vka4	gr_vka4	log	705	0	1
gr_vka3	gr_vka3	log	705	0	1
cn_vka8	cn_vka8	log	1	0	1
gr_hk4	gr_hk4	log	705	0	1
pp_sy1	pp_sy1	log	32	0	0.243038
cn_sy8	cn_sy8	log	1	0	0.243038
cn_ss6	cn_ss6	log	1	0	1
cn_prsity8	cn_prsity8	log	1	0	0.176091
cn_strt7	cn_strt7	log	1	0	0.0211893
pp_prsity2	pp_prsity2	log	32	0	0.176091
pp_rech0	pp_rech0	log	32	0	0.0413927
cn_strt6	cn_strt6	log	1	0	0.0211893
gr_strt4	gr_strt4	log	705	0	0.0211893
pp_hk1	pp_hk1	log	32	0	1
cn_rech5	cn_rech5	log	1	-0.39794	-0.09691
gr_rech3	gr_rech3	log	705	0.00701	0.0413927
welflux_k02	welflux_k02	log	6	0	1
gr_hk3	gr_hk3	log	705	0	1
0	9 m.o	±08	, 00	V	_

	lower bound	$\operatorname{standard}$	${\tt deviation}$
gr_strt3	-0.0222764		0.0108664
gr_sy5	-0.60206		0.211275
pp_strt0	-0.0222764		0.0108664
pp_hk2	-1		0.5
cn_prsity6	-0.30103		0.11928
cn_sy7	-0.60206		0.211275
gr_ss4	-1		0.5
pp_sy0	-0.60206		0.211275
gr_rech2	-0.0457575		0.0217875
strk	-2		1
cn_strt8	-0.0222764		0.0108664
pp_sy2	-0.60206		0.211275
cn_hk7	-1		0.5
pp_rech1	-0.0457575		0.0217875
pp_strt2	-0.0222764		0.0108664
cn_vka6	-1		0.5
pp_vka1	-1		0.5
cn_ss8	-1		0.5
cn_ssc cn_rech4	-0.09691		0.0440228
gr_prsity5	-0.30103		0.11928
pp_hk0	-1		0.11325
cn_ss7	-1		0.5
	-1		0.5
pp_ss2	-0.60206		0.5
gr_sy4	-0.30103		0.211273
cn_prsity7			0.11928
gr_prsity3	-0.30103		
cn_vka7	-1		0.5
pp_ss1	-1		0.5
pp_prsity0	-0.30103		0.11928
pp_ss0	-1		0.5
gr_prsity4	-0.30103		0.11928
gr_ss5	-1		0.5
gr_vka5	-1		0.5
pp_vka2	-1		0.5
gr_strt5	-0.0222764		0.0108664
cn_sy6	-0.60206		0.211275
pp_prsity1	-0.30103		0.11928
gr_ss3	-1		0.5
gr_sy3	-0.60206		0.211275
cn_hk8	-1		0.5
drncond_k00	-1		0.5
gr_vka4	-1		0.5
gr_vka3	-1		0.5
cn_vka8	-1		0.5

```
gr_hk4
                                        0.5
                      -1
               -0.60206
                                   0.211275
pp_sy1
cn_sy8
               -0.60206
                                   0.211275
cn_ss6
                     -1
                                        0.5
               -0.30103
                                    0.11928
cn_prsity8
cn_strt7
             -0.0222764
                                  0.0108664
pp_prsity2
               -0.30103
                                    0.11928
             -0.0457575
pp_rech0
                                  0.0217875
cn_strt6
             -0.0222764
                                  0.0108664
             -0.0222764
                                  0.0108664
gr_strt4
                     -1
pp_hk1
                                        0.5
cn_rech5
                     -1
                                   0.225772
                                  0.0217875
gr_rech3
             -0.0457575
                                        0.5
welflux_k02
                     -1
                      -1
                                        0.5
gr_hk3
gr_hk5
                                        0.5
                     -1
```

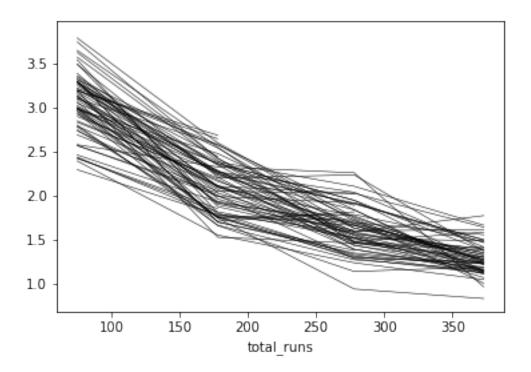
[65 rows x 7 columns]

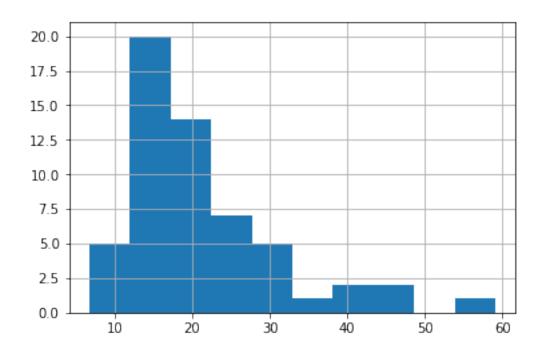
Should we fix either PP or grids?

```
In [5]: 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
```

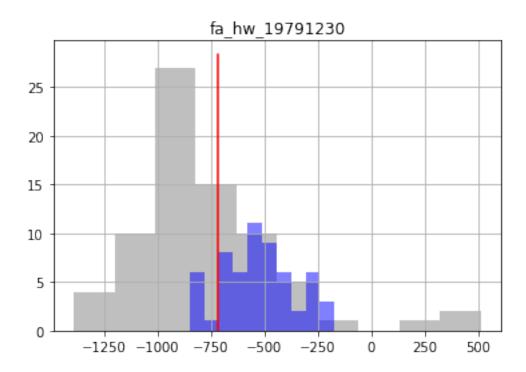
### 1.1.1 Run PESTPP-IES in original mode and post process

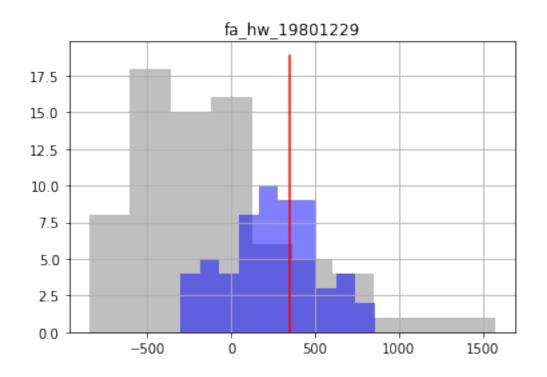
```
In [6]: #pst.pestpp_options = {}
    pst.pestpp_options["ies_num_reals"] = 75
    pst.pestpp_options["ies_par_en"] = "prior.jcb"
    pst.pestpp_options["ies_bad_phi_sigma"] = 1.75
    pst.pestpp_options["overdue_giveup_fac"] = 10.0
    pst.control_data.noptmax = 3
In [7]: pst.write(os.path.join(t_d, "freyberg_ies.pst"))
noptmax:3, npar_adj:14819, nnz_obs:14
In [8]: pyemu.os_utils.start_slaves(t_d, "pestpp-ies", "freyberg_ies.pst", num_slaves=num_workers
    A cheap phi progress plot
```

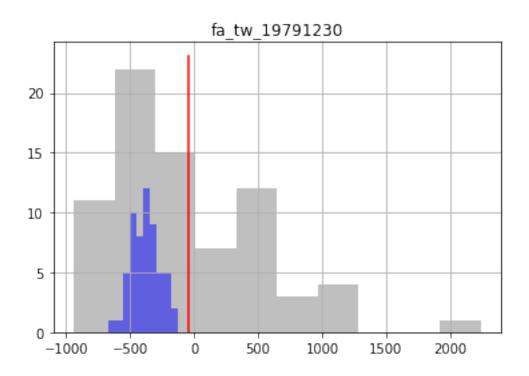


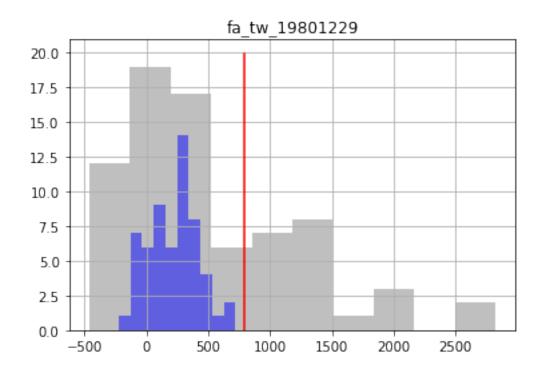


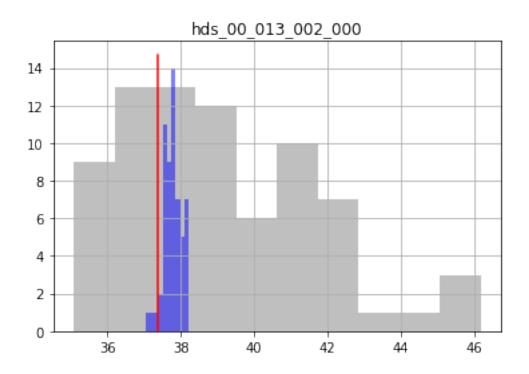
Plot forecast prior and posterior histograms with "truth" (red line)

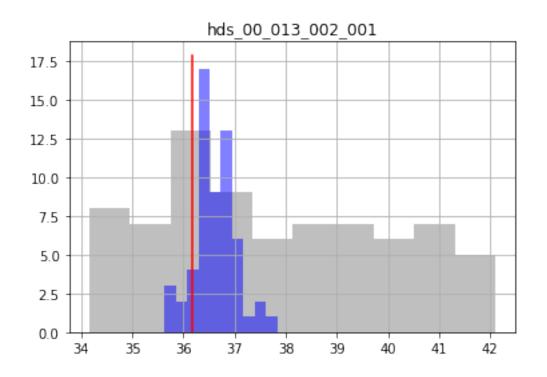


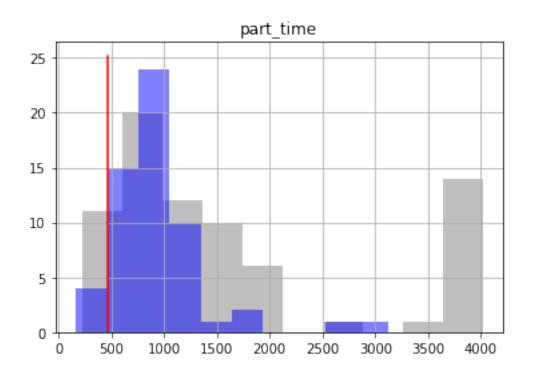


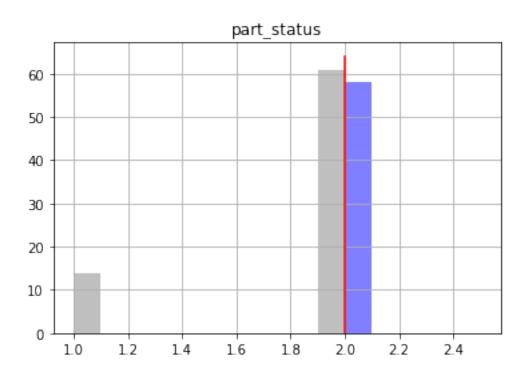








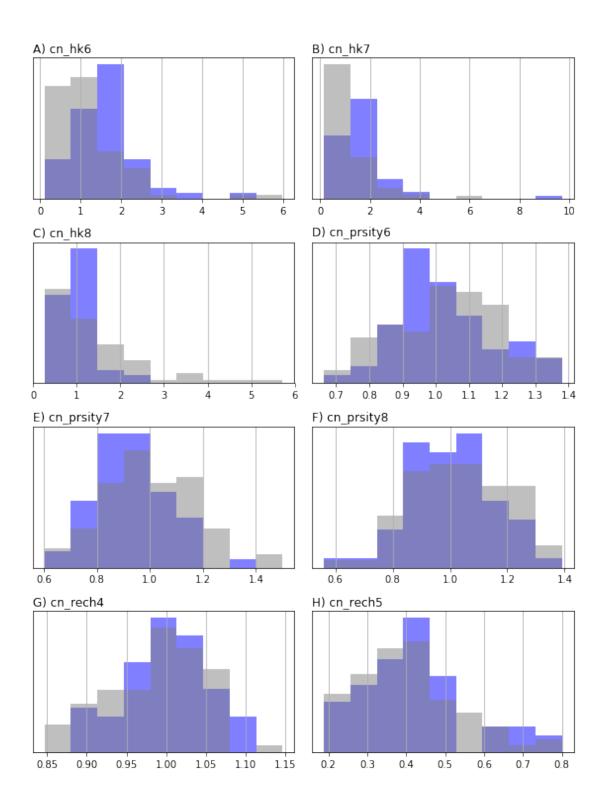


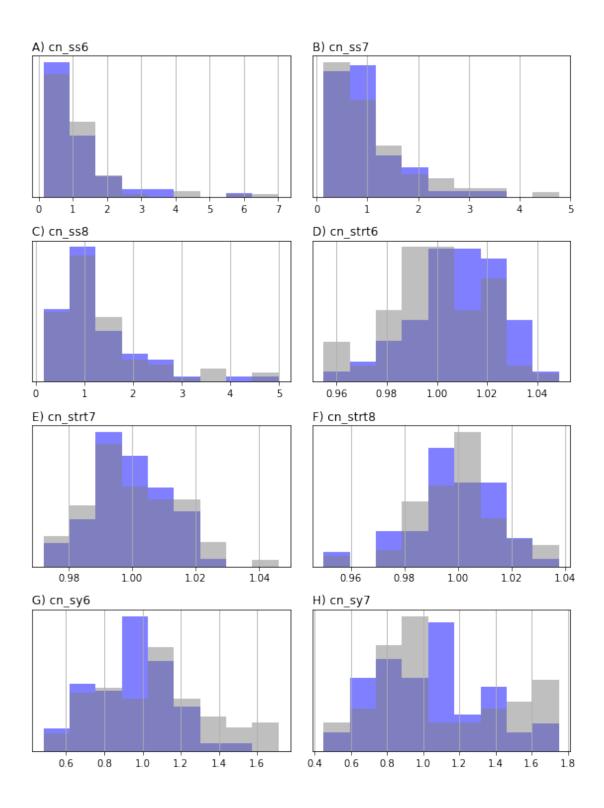


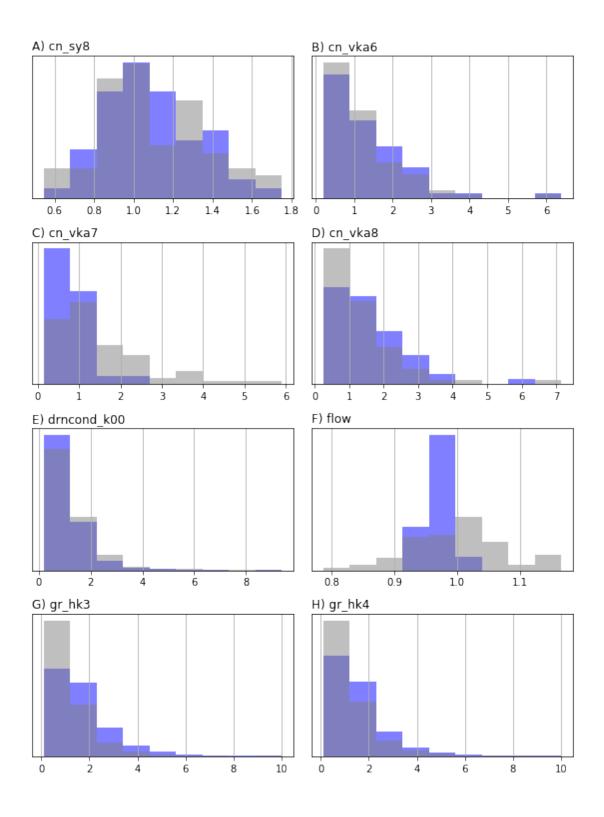
### Plot parameter histograms by group

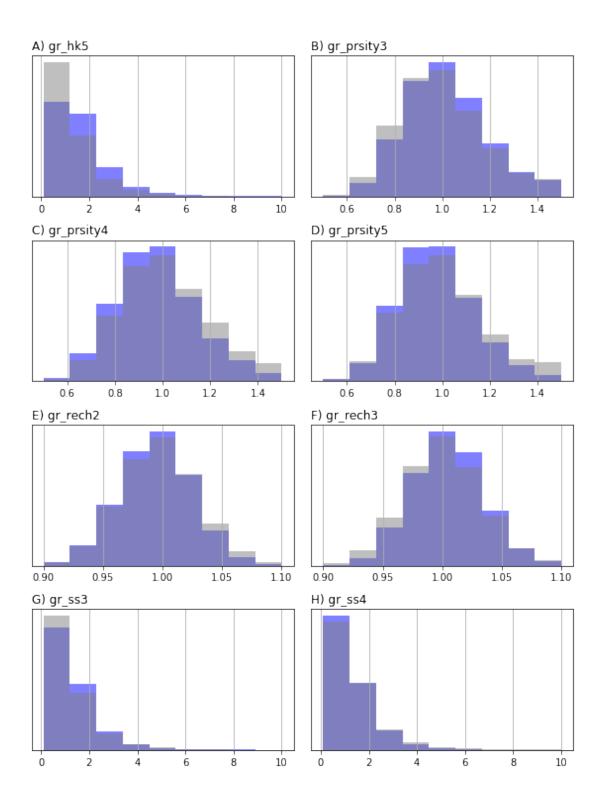
/Users/jeremyw/miniconda3/lib/python3.5/site-packages/IPython/core/interactiveshell.py:2785: Dinteractivity=interactivity, compiler=compiler, result=result)

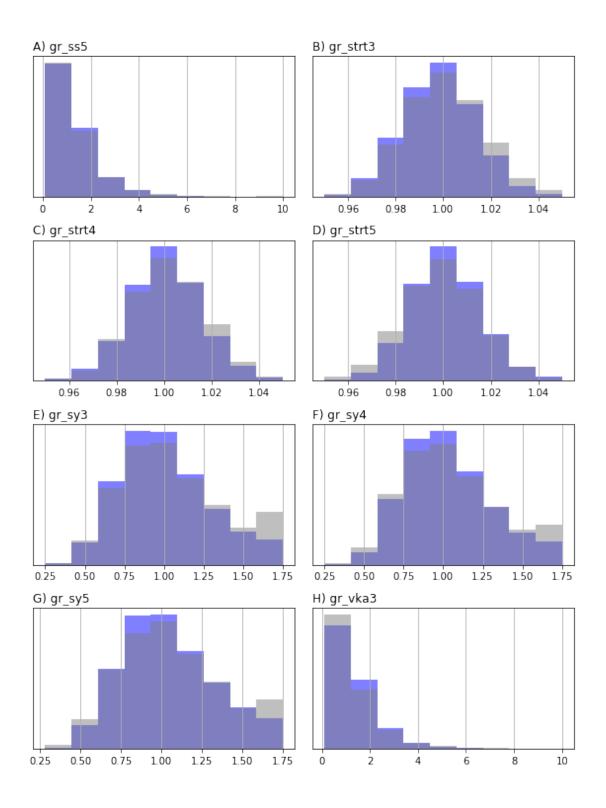
<Figure size 576x756 with 0 Axes>

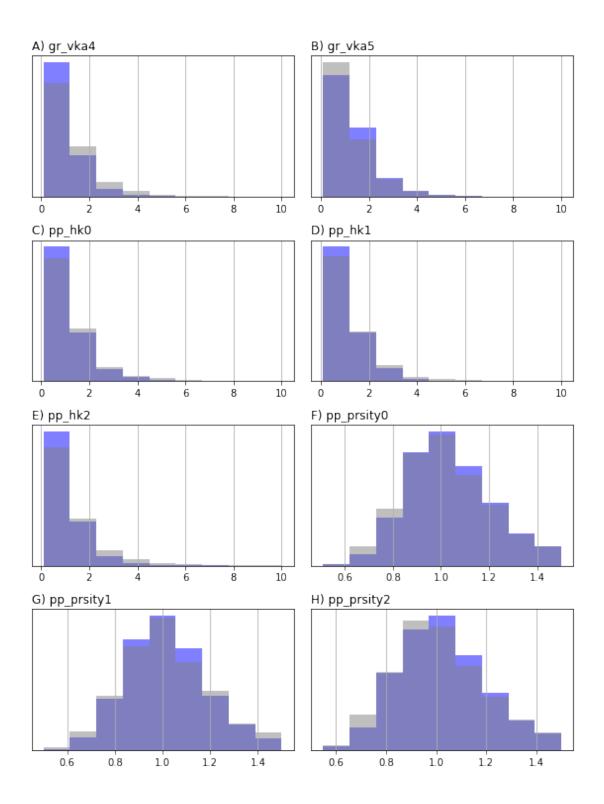


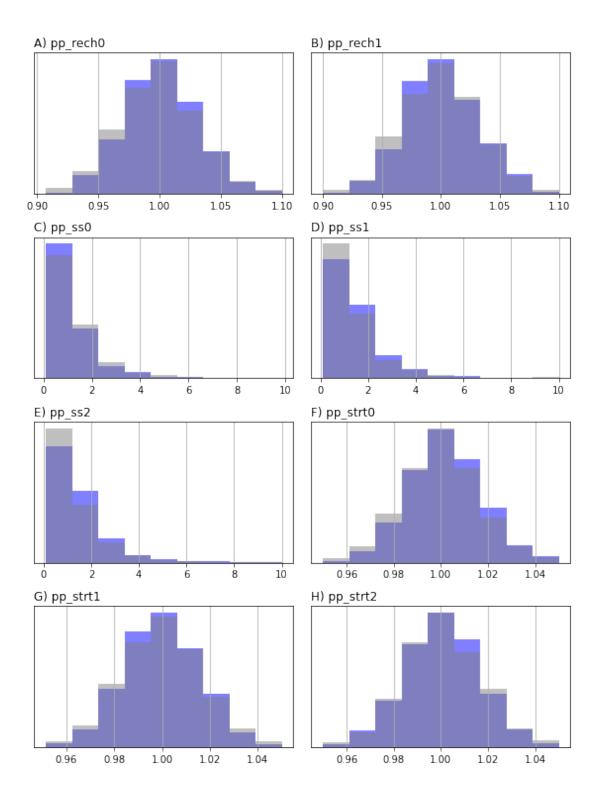


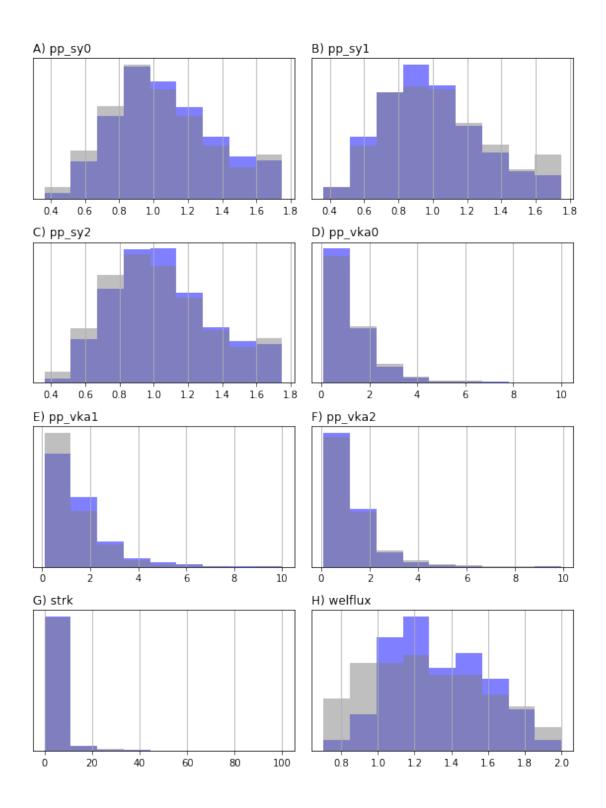












# A) welflux\_k02

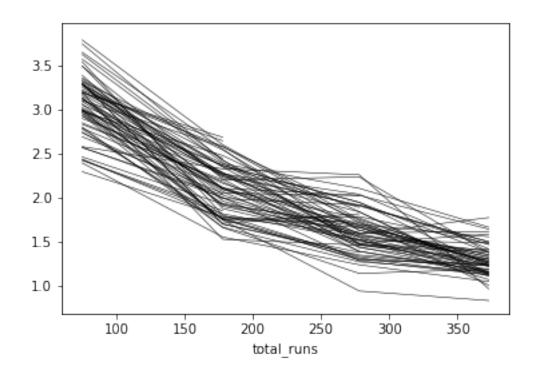
```
# pe_pr.loc[:,li] = pe_pr.loc[:,li].apply(np.log10)
# pe_pr.shape
```

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

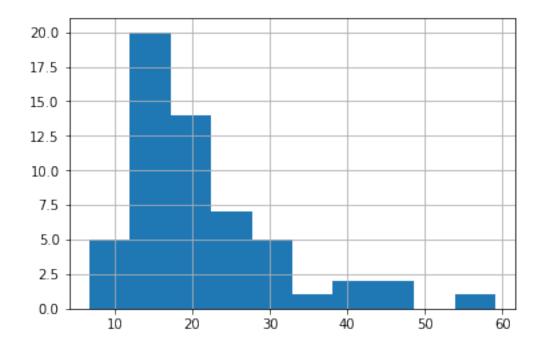
Now let's add some localization. The obvious stuff is temporal - scenario parameters can't influence historic observations (and the inverse is true) so let's tell PESTPP-IES about this. Also, should porosity be adjusted at all given the observations we have???

```
In [13]: 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[13]: ['cn_prsity6',
          'gr_prsity5',
          'cn_prsity7',
          'gr_prsity3',
          'pp_prsity0',
          'gr_prsity4',
          'pp_prsity1',
          'cn_prsity8',
          'pp_prsity2',
          'gr_rech3',
          'pp_rech1',
          'cn_rech5',
          'welflux_001']
In [14]: 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 [15]: 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=num_worker
noptmax:3, npar_adj:14819, nnz_obs:14
In [16]: phi = pd.read_csv(os.path.join(m_d, "freyberg_ies.phi.actual.csv"),index_col=0)
         phi.index = phi.total_runs
```

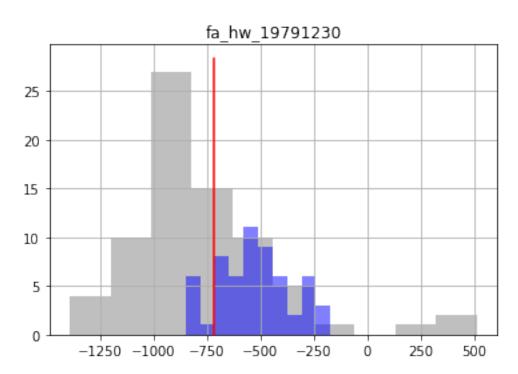
```
phi.iloc[:,6:].apply(np.log10).plot(legend=False,lw=0.5,color='k')
plt.show()
phi.iloc[-1,6:].hist()
```

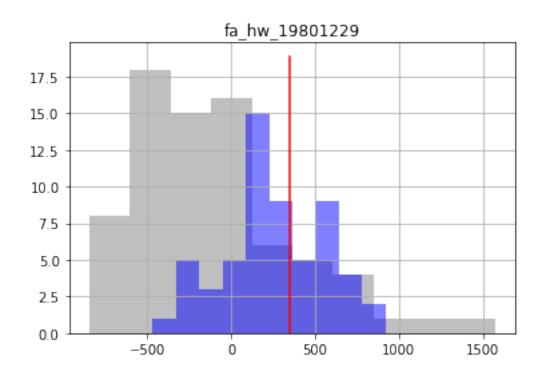


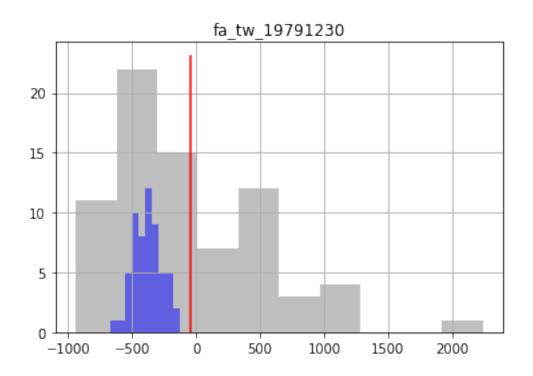
Out[16]: <matplotlib.axes.\_subplots.AxesSubplot at 0x182a26ceb8>

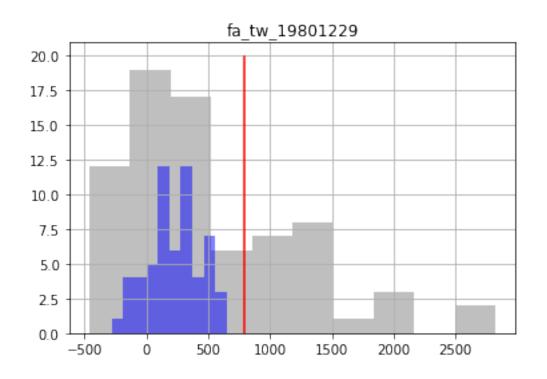


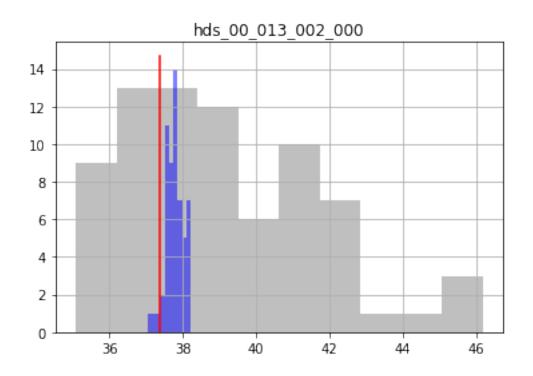
```
In [17]: oe_pr = pd.read_csv(os.path.join(m_d, "freyberg_ies.0.obs.csv"),index_col=0)
    oe_pt = pd.read_csv(os.path.join(m_d, "freyberg_ies.{0}.obs.csv".format(pst.control_data)
    obs = pst.observation_data
    fnames = pst.pestpp_options["forecasts"].split(",")
    for forecast in fnames:
        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()
```

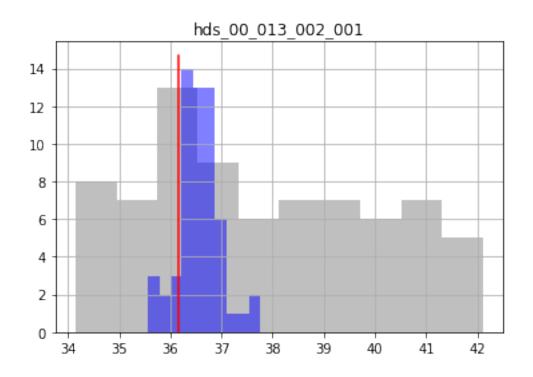


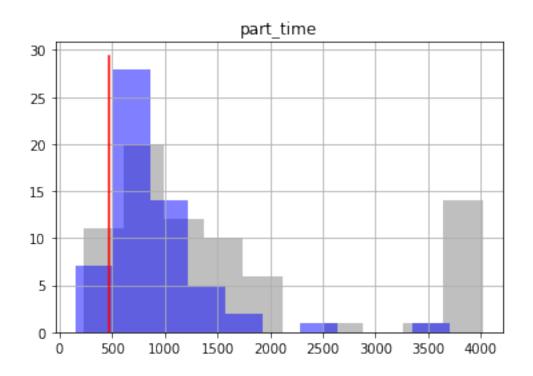


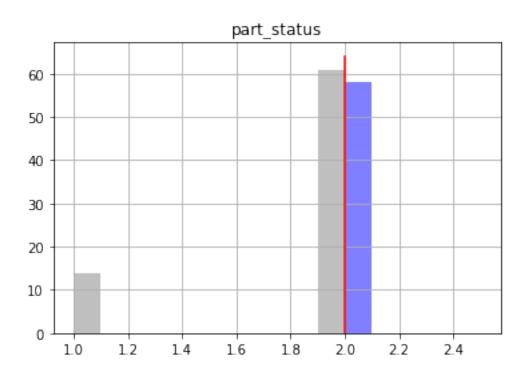








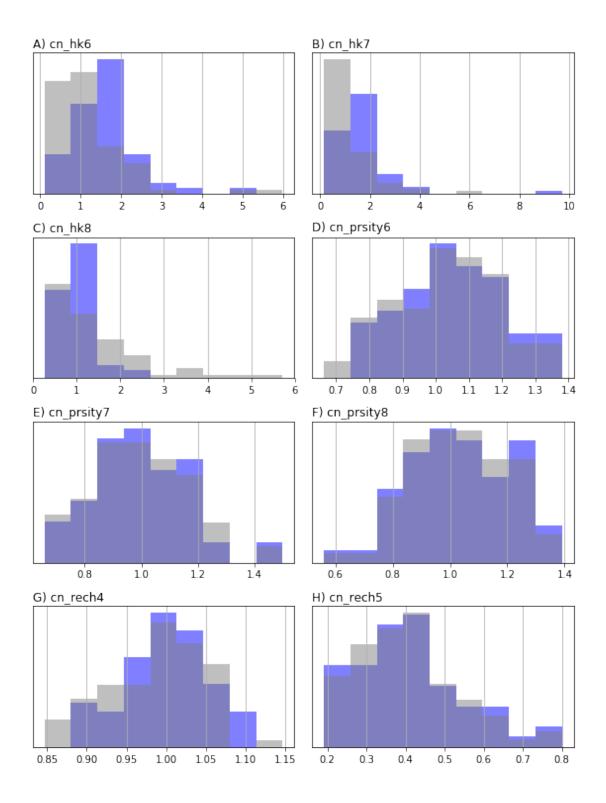


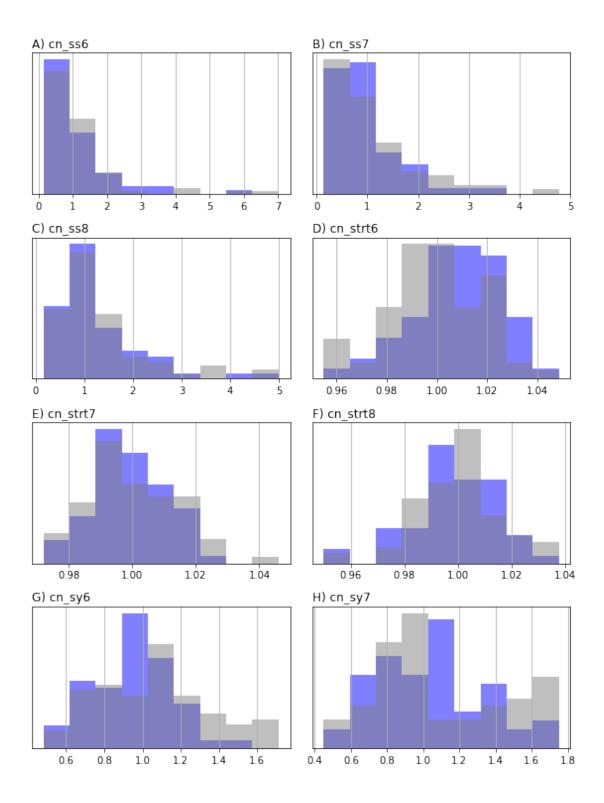


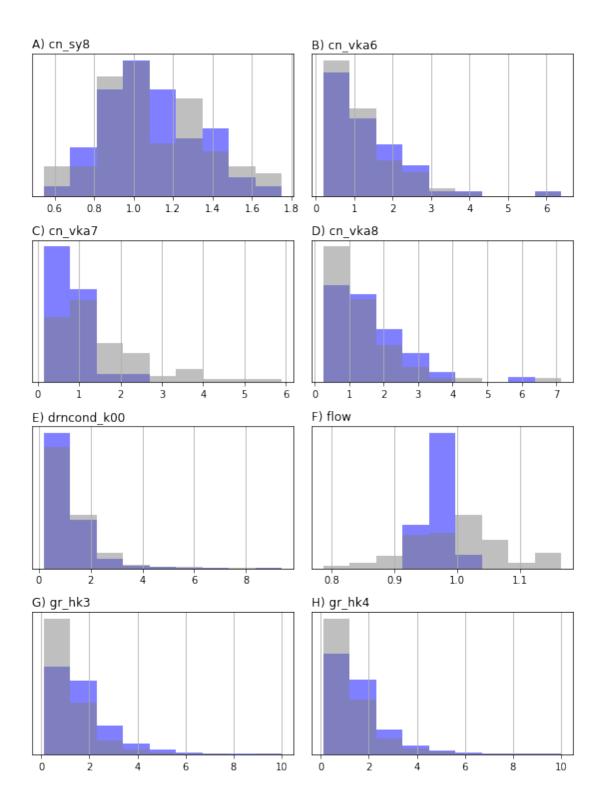
/Users/jeremyw/miniconda3/lib/python3.5/site-packages/IPython/core/interactiveshell.py:2785: Dinteractivity=interactivity, compiler=compiler, result=result)

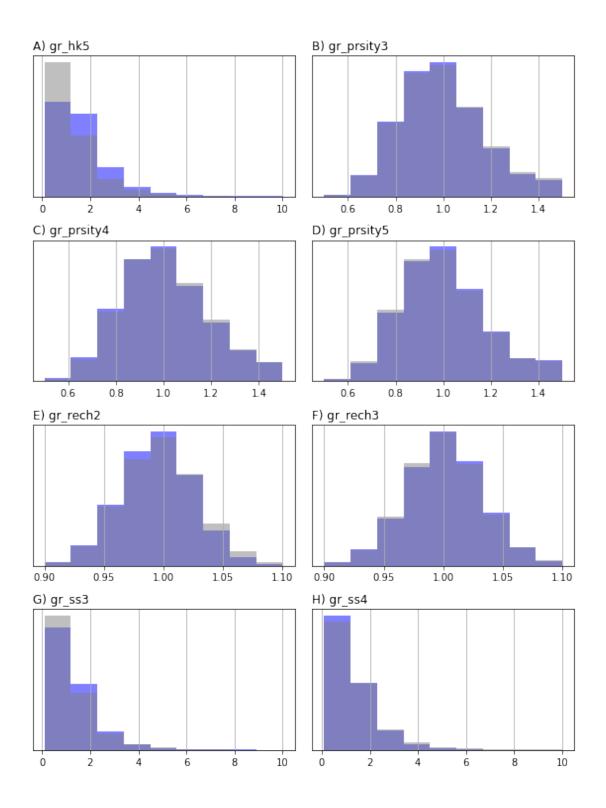
(75, 14819) (58, 14819)

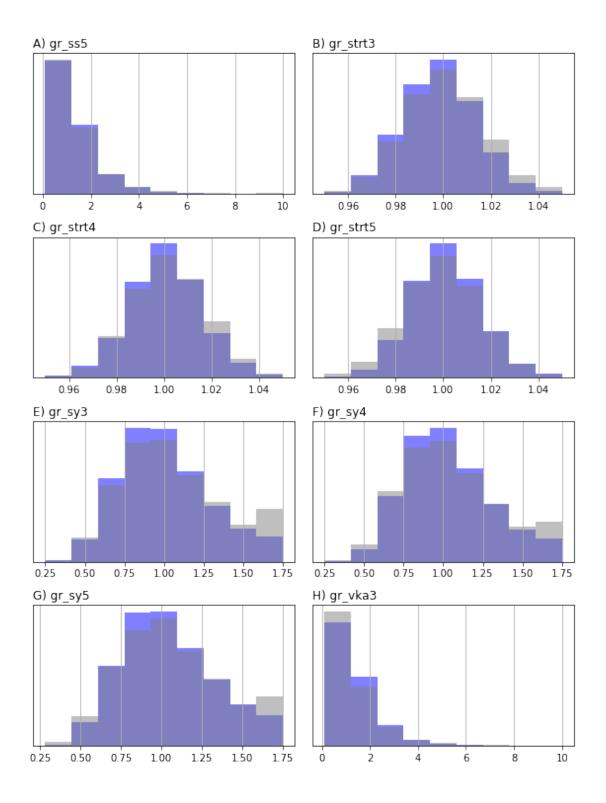
<Figure size 576x756 with 0 Axes>

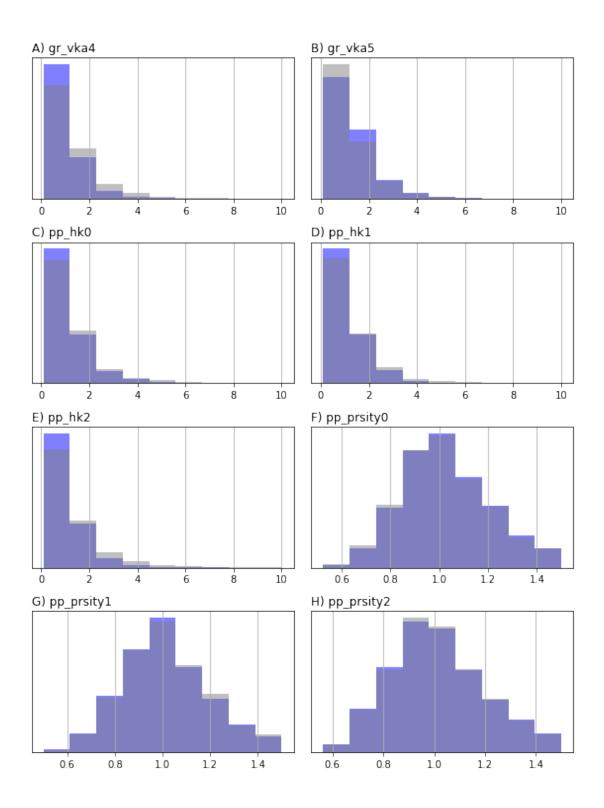


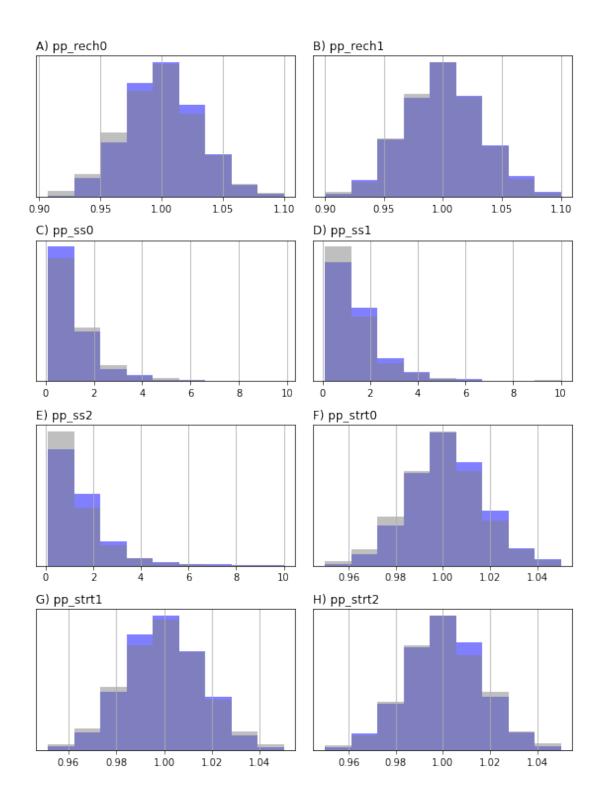


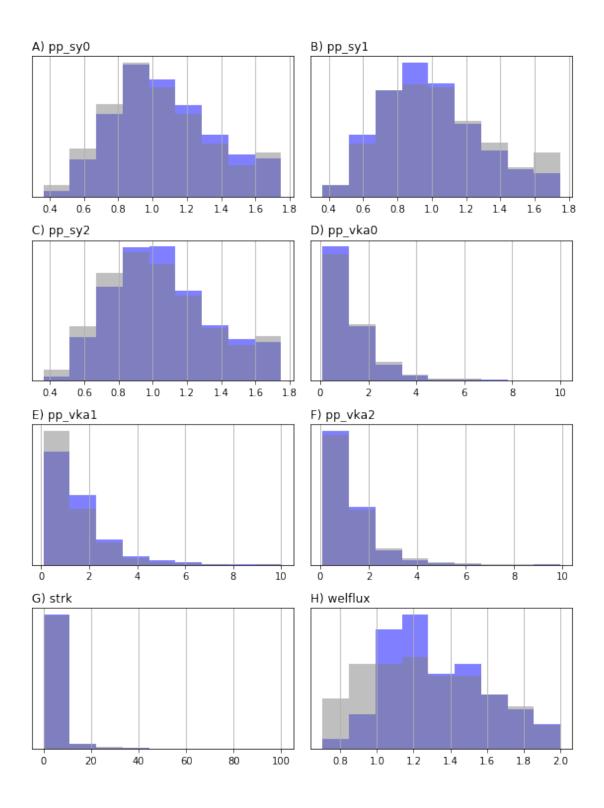


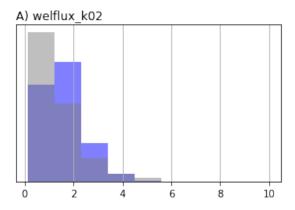










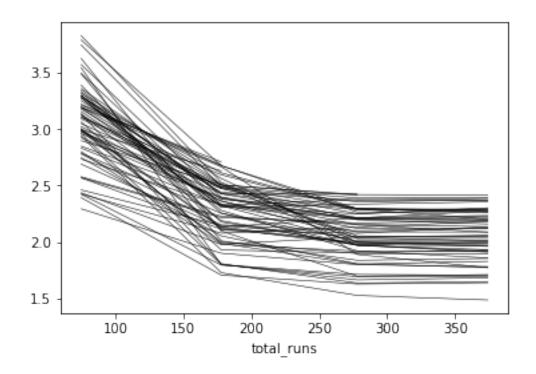


## 1.1.3 PESTPP-IES with par-by-par distance based localization

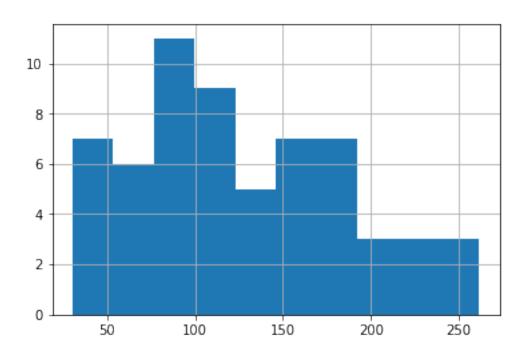
```
In [19]: m = flopy.modflow.Modflow.load("freyberg.nam",model_ws="template")
```

```
In [20]: 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 [21]: 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
```

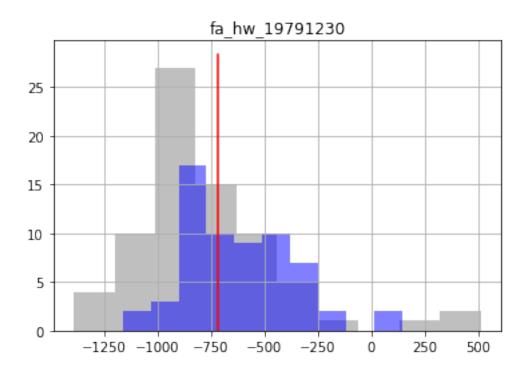
```
\#spars = par.loc[par.parnme.apply(lambda x: "ss" in x or "sy" in x),"parnme"]
         \#loc.loc[:,spars] = 0.0
         loc.sum(axis=1)
hds_00_002_009_000 0.46382978723404256 0.46875
hds_00_002_015_000 0.4794326241134752 0.5
hds_00_003_008_000 0.43829787234042555 0.34375
hds_00_009_001_000 0.3304964539007092 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 [21]: 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 [22]: 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"))
noptmax:3, npar_adj:14819, nnz_obs:14
In [23]: pyemu.os_utils.start_slaves(t_d,"pestpp-ies","freyberg_ies.pst",num_slaves=num_worker
In [24]: 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()
```

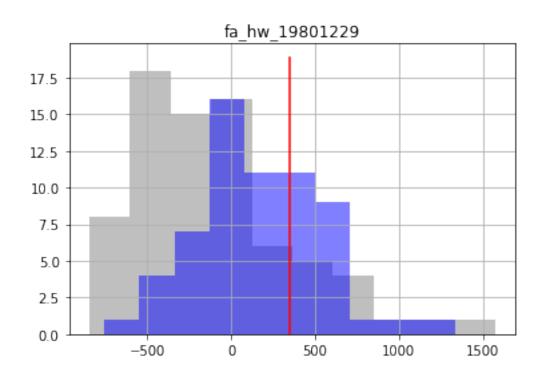


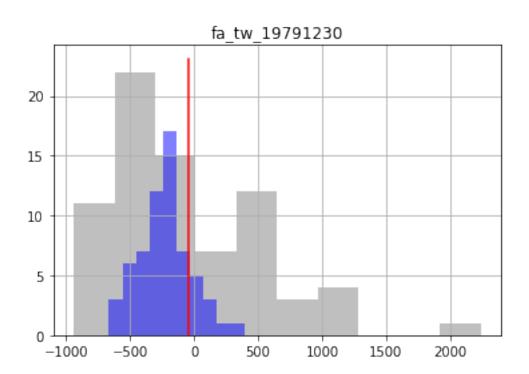
Out[24]: <matplotlib.axes.\_subplots.AxesSubplot at 0x10fef7da0>

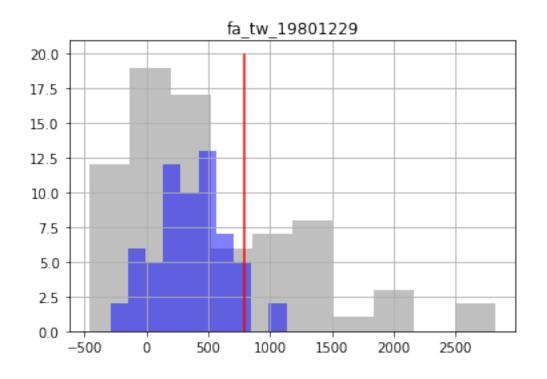


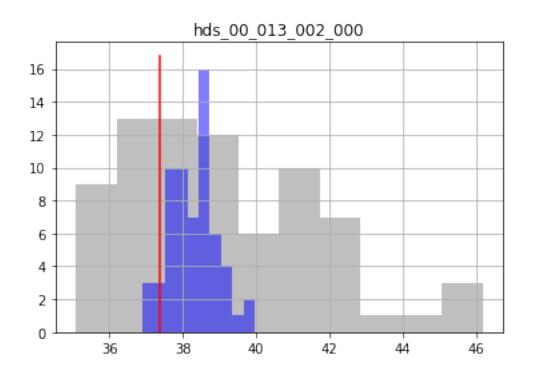
```
In [25]: oe_pr = pd.read_csv(os.path.join(m_d, "freyberg_ies.0.obs.csv"),index_col=0)
    oe_pt = pd.read_csv(os.path.join(m_d, "freyberg_ies.{0}.obs.csv".format(pst.control_data)
    obs = pst.observation_data
    fnames = pst.pestpp_options["forecasts"].split(",")
    for forecast in fnames:
        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()
```

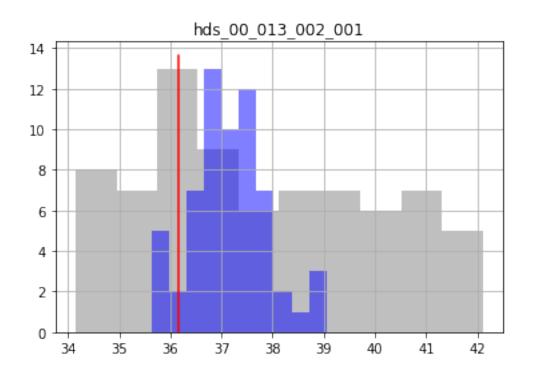


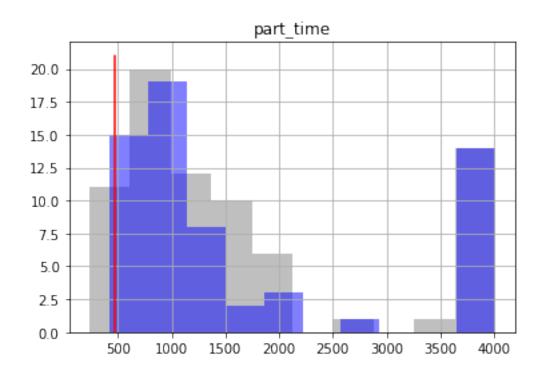


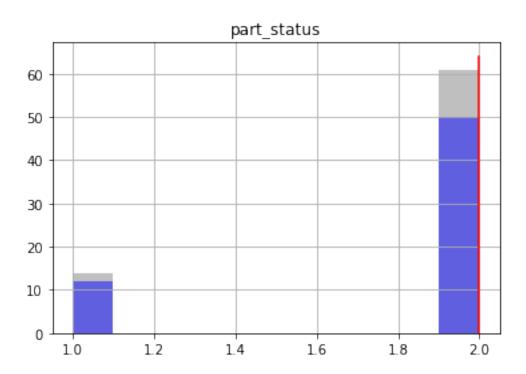












/Users/jeremyw/miniconda3/lib/python3.5/site-packages/IPython/core/interactiveshell.py:2785: Dinteractivity=interactivity, compiler=compiler, result=result)

<Figure size 576x756 with 0 Axes>

