Instructions for generating plots shown in paper, "The 'ABC-DA' system (v1.4): a variational data assimilation system for convective scale research with a study of the impact of a balance constraint"

January 17, 2020

Further guidance on downloading, compiling, and running the software is available in the documentation on github (DOI: 10.5281/zenodo.3531926). The mentioned document also shows how the python plotting code is accessed.

1 Figure 1

This is a schema, and so doesn't require production of any results.

2 Figure 2

1. This requires the control variable transform (CVT) to first be calibrated. Make directory to contain *CVT.nc* file (call *Master_Calibration*), and enter this directory.

2. Make directory inside *Master_Calibration* (call *Master_Calibration_stage1*) and enter this directory.

3. Generate ensemble to be used for calibrating the CVT from given UM file (*Member001.nc* inside directory */home/data/UMdir* in this example). Run *Master_Calibration.out* with the following namelist file present (*UserOptions.nl*). See documentation, §4.4.1.

```
&UserOptions
! Reading and processing UM data
! ---------------------------------
A                        = 0.02,
B                        = 0.01,
C                        = 1.0E4,
dt                       = 4.0,
Adv_tracer               = .TRUE.,
runlength                = 3600.0,
CalibRunStage            = 1,
NEns                     = 1,
EnsDirs(1)               = '/home/data/UMdir',
NEnsMems                 = 1,
NNMC                     = 0,
Nlats                    = 260,
latindex(1)              = 11,
latindex(2)              = 12,
latindex(3)              = 13,
latindex(4)              = 14,
latindex(5)              = 15,
latindex(6)              = 16,
latindex(7)              = 17,
latindex(8)              = 18,
latindex(9)              = 19,
latindex(10)             = 20,
latindex(11)             = 21,
```

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latindex(12)          = 22,
latindex(13)          = 23,
latindex(14)          = 24,
latindex(15)          = 25,
latindex(16)          = 26,
latindex(17)          = 27,
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latindex(19)          = 29,
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latindex(22)          = 32,
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latindex(24)          = 34,
latindex(25)          = 35,
latindex(26)          = 36,
latindex(27)          = 37,
latindex(28)          = 38,
latindex(29)          = 39,
latindex(30)          = 40,
latindex(31)          = 41,
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latindex(68)          = 78,
latindex(69)          = 79,
latindex(70)          = 80,
latindex(71)          = 81,
latindex(72)          = 82,
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latindex(73)          = 83,
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latindex(129)         = 139,
latindex(130)         = 140,
latindex(131)         = 141,
latindex(132)         = 142,
latindex(133)         = 143,
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latindex(192)          = 202,
latindex(193)          = 203,
latindex(194)          = 204,
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latindex(252)          = 262,
latindex(253)          = 263,
latindex(254)          = 264,
latindex(255)          = 265,
```

```
latindex(256)            = 266,
latindex(257)            = 267,
latindex(258)            = 268,
latindex(259)            = 269,
latindex(260)            = 270,
BoundSpread              = 100,
datadirABCfcs            = '.',
datadirCVT               = '..',
CVT_file                 = 'CVT.nc',
CVT%CVT_order            = 1,
CVT%CVT_param_opt_gb     = 1,
CVT%CVT_param_opt_hb     = 1,
CVT%CVT_param_opt_ab     = 2,
CVT%CVT_param_opt_reg    = 1,
CVT%CVT_vert_opt_sym     = 1,
CVT%CVT_stddev_opt       = 2
/
```

4. Make directory inside *Master_Calibration* (call *Master_Calibration_stage2*) and enter this directory.

5. Generate ensemble mean state, and perturbations from this ensemble. Run *Master_Calibration.out* with the following namelist file present (*UserOptions.nl*). See documentation, §4.4.2.

```
&UserOptions
! Generating ensemble perturbations from ensemble forecasts
! ----------------------------------------------------------
CalibRunStage      = 2,
NEns               = 1,
NEnsMems           = 1,
NNMC               = 0,
Nlats              = 260,
datadirABCfcs      = '../Master_Calibration_stage1',
datadirABCperts    = '.',
datadirCVT         = '../',
CVT_file           = 'CVT.nc'
/
```

6. Make directory inside *Master_Calibration* (call *Master_Calibration_stage3*) and enter this directory.

7. Generate vertical regression matrix. Run *Master_Calibration.out* with the following namelist file present (*UserOptions.nl*). See documentation, §4.4.3.

```
&UserOptions
! Generate vertical regression matrix
! -----------------------------------
CalibRunStage      = 3,
NEns               = 1,
NEnsMems           = 1,
NNMC               = 0,
Nlats              = 260,
datadirRegression  = '.',
datadirABCperts    = '../Master_Calibration_stage2',
datadirCVT         = '..',
CVT_file           = 'CVT.nc'
/
```

8. To plot figure 2(c), edit the python program *PlotRegressionMatrices.py* to set *datadirCVT* to *Master_Calibration*, and run the python program.

9. Make directory inside *Master_Calibration* (call *Master_Calibration_stage4*) and enter this directory.

10. Generate ensemble perturbations in terms of parameters. Run *Master_Calibration.out* with the following namelist file present (*UserOptions.nl*). See documentation, §4.4.4.

```
&UserOptions
! Generate parameter perturbations
! ------------------------------------------
CalibRunStage      = 4,
NEns               = 1,
NEnsMems           = 1,
NNMC               = 0,
Nlats              = 260,
datadirABCperts    = '../Master_Calibration_stage2',
datadirConParams   = '.',
datadirCVT         = '..',
CVT_file           = 'CVT.nc',
/
```

11. To plot Figs. 2(a,b,d), edit the python program *Plot_rp_pre+post_regress.py* to set *data_dir_stage2* to *Master_Calibration/Master_Calibration_stage2* and *data_dir_stage4* to *Master_Calibration/Master_Calibration_st* and run the python program.

3 Figure 3

1. Make directory inside *Master_Calibration* (call *Master_Calibration_stage5*) and enter this directory.

2. Generate spatial transform data (the remaining part of the calibration step). Run *Master_Calibration.out* with the following namelist file present (*UserOptions.nl*). See documentation, §4.4.5.

```
&UserOptions
! Calibrate spatial transforms
! ------------------------------------
CalibRunStage      = 5,
NEns               = 1,
NEnsMems           = 1,
NNMC               = 0,
Nlats              = 260,
datadirABCperts    = '../Master_Calibration_stage2',
datadirConParams   = '../Master_Calibration_stage4',
datadirCVT         = '..',
CVT_file           = 'CVT.nc'
/
```

3. Edit the python program *PlotCVT.py* to set *data_dir_CVT* to *Master_Calibration*, and run the python program.

4. This can be repeated for different experiment configurations to get the different lines in panel (c) of the paper.

4 Figure 4

1. This is also output from *PlotCVT.py* as run for Fig. 3.

2. This can be repeated for different experiment configurations to get the different lines in panel (c) of the paper.

5 Figure 5

1. This is also output from *PlotCVT.py* as run for Fig. 3.

6 Figure 6

1. This plot requires the same data as used for Fig. 5, plus knowledge of the gravity wave speeds (found from a linear analysis). Run a linear analysis of the model by first creating a directory *Master_Linear_Analysis* (in the same place as directory *Master_Calibration*) and enter this directory. Run *Master_Linear_Analysis.out* with the following namelist file present (*UserOptions.nl*). See documentation, §4.3.

```
&UserOptions
! Linear analysis of ABC model equations
! -----------------------------------------
  datadirLinearAnal,          = '.'
  A                           = 0.02
  B                           = 0.01
  C                           = 1.0E4
/
```

2. Compile the c++ program RossbyRadius.cpp (contained in the same directory as the python plotting code, note the libraries that are required):

```
g++ -I/usr/include RossbyRadius.cpp -o RossbyRadius.out -L/usr/lib -lnetcdf_c++ -lnetc
```

3. Run this code as follows from the command line inside directory *Master_Linear_Analysis*:

```
./RossbyRadius.out ../Master_Calibration .
```

4. To plot Fig. 6, edit the python program *Plot_horizvars_unbalrho+Rossby.py* to set *CVT_file* to *Master_Calibration* and *lengths_file* to *Master_Linear_Analysis/VerticalModeCharacteristics.dat* and run the python program.

7 Figure 7

1. Make a directory *Master_ImpliedCovs* (in the same place as directory *Master_Calibration*) and enter this directory. Run *Master_ImpliedCov.out* with the following namelist file present (*UserOptions.nl*). See documentation, §4.6.

```
&UserOptions
! Compute implied covariances
! -------------------------------
  datadirImpliedCov           = '.',
  datadirCVT                  = '../Master_Calibration',
  CVT_file                    = 'CVT.nc',
  datadirABCfcs               = '../Master_Calibration/Master_Calibration_stage1',
  LS_file                     = 'FC_Ens001_Item001.nc',
  ImplCov_npoints             = 1
  longindex(1)                = 180
  levindex(1)                 = 25
/
```

2. To plot panels (a), (b), and (c) of Fig. 7, edit the python program *Plot_Covs.py* to set *plot_raw_covs* to *False*, *plot_implied_covs* to *True*, *data_dir_ImpliedCovs* to *Master_ImpliedCovs*, *longindex* to [179], and *levindex* = [24], and run the python program. Note that the *longindex* and *levindex* are *longindex*(1)-1 and *levindex*(1)-1 respectively.

3. This can be repeated for different experiment configurations to get the rows 2 and 3 of Fig. 7 in the paper.

4. Make directory *Master_RawCov* (in the same place as directory *Master_Calibration*) and enter this directory. Run *Master_RawCov.out* with the following namelist file present (*UserOptions.nl*). See documentation, §4.7.

```
&UserOptions
! Compute raw covariances
! ------------------------
  datadirRawCov        = '.'
  datadirABCperts      = '../Master_Calibration/Master_Calibration_stage2'
  Nens                 = 1
  NensMems             = 1
  Nlats                = 260
  ImplCov_npoints      = 1
  longindex(1)         = 180
  levindex(1)          = 25
/
```

5. To plot panels (j), (k), and (l) of Fig. 7, edit the python program *Plot_Covs.py* to set *plot_raw_covs* to *True*, *plot_implied_covs* to *False*, *data_dir_RawCovs* to *Master_RawCovs*, *Nens* to 1, *NEnsMems* to 260, *longindex* to [179], and *levindex* = [24], and run the python program. Note that the *longindex* and *levindex* are *longindex*(1)-1 and *levindex*(1)-1 respectively.

8 Figure 8

This is a schema, and so doesn't require production of any results.

9 Figure 9

1. Make an ABC-style initial state (in order to generate synthetic observations and to measure errors from). Make a directory *Master_PrepareABC_InitState* (in the same place as directory *Master_Calibration*) and enter this directory.

2. Run *Master_PrepareABC_InitState.out* with the following namelist file present (*UserOptions.nl*). See documentation, §4.1.

```
&UserOptions
! Master_PrepareABC_InitState
! ----------------------------
  Init_ABC_opt         = 3
  datadirUM            = '/home/data/UMdir'
  init_um_file         = 'Member0001.nc'
  datadirABC_out       = '.'
  init_ABC_file        = 'ABC_InitialConds.nc'
  latitude             = 102
  Regular_vert_grid    = .TRUE.
  Adv_tracer           = .TRUE.
  gravity_wave_switch  = .FALSE.
  f                    = 1.0E-4
  A                    = 0.02
  B                    = 0.01
  C                    = 1.0E4
  BoundSpread          = 100.
  press_source_x       = 200
  press_source_z       = 6
  press_amp            = 0.005
  x_scale              = 120
  z_scale              = 14
/
```

3. Make a short forecast from this initial state to spin-up characteristics of the ABC model. Make a directory *Master_RunNLModel* (in the same place as directory *Master_Calibration*) and enter this directory.

4. Run *Master_RunNLModel.out* with the following namelist file present (*UserOptions.nl*). See documentation, §4.2.

```
&UserOptions
! Running ABC model
! ------------------
  datadirABC_in                = '../Master_PrepareABC_InitState'
  init_ABC_file                = 'ABC_InitialConds.nc'
  datadirABC_out               = '.'
  output_ABC_file              = 'Truth.nc'
  diagnostics_file             = 'ABC_Diagnostics.dat'
  runlength                    = 7200.0
  ndumps                       = 9
  dt                           = 4.0
  Lengthscale_diagnostics      = .FALSE.
  A                            = 0.02
  B                            = 0.01
  C                            = 1.0E4
  Adv_tracer                   = .TRUE.
/
```

5. Specify the observation network. Make directory *Master_MakeBgObs_ObsNetwork* (in the same place as directory *Master_Calibration*) and enter this directory.

6. Run *Master_MakeBgObs.out* with the following namelist file present (*UserOptions.nl*). See documentation, §4.8.

```
&UserOptions
! Specification of observation network
! ------------------------------------
  Generate_mode                = 1
  ObsSpec%year0                = 2010
  ObsSpec%month0               = 1
  ObsSpec%day0                 = 1
  ObsSpec%hour0                = 0
  ObsSpec%min0                 = 0
  ObsSpec%sec0                 = 0
  ObsSpec%NumBatches           = 7
  datadir_ObsSpec              = '.'
  ObsSpec_file                 = 'ObsSpec.dat'
! ------------------------------
  ObsSpec%batch(1)             = 1
  ObsSpec%seconds(1)           = 0
  ObsSpec%ob_of_what(1)        = 4          ! rp
  ObsSpec%NumObs_long(1)       = 18
  ObsSpec%NumObs_height(1)     = 20
  ObsSpec%long_min(1)          = 10.0
  ObsSpec%long_max(1)          = 530000.0
  ObsSpec%height_min(1)        = 1.0
  ObsSpec%height_max(1)        = 12000.0
  ObsSpec%stddev(1)            = 0.0015
! ------------------------------
  ObsSpec%batch(2)             = 2
  ObsSpec%seconds(2)           = 600
  ObsSpec%ob_of_what(2)        = 4          ! rp
  ObsSpec%NumObs_long(2)       = 18
  ObsSpec%NumObs_height(2)     = 20
  ObsSpec%long_min(2)          = 10.0
  ObsSpec%long_max(2)          = 530000.0
  ObsSpec%height_min(2)        = 1.0
```

```
    ObsSpec%height_max(2)      = 12000.0
    ObsSpec%stddev(2)          = 0.0015
!  -------------------------------------
    ObsSpec%batch(3)           = 3
    ObsSpec%seconds(3)         = 1200
    ObsSpec%ob_of_what(3)      = 4          ! rp
    ObsSpec%NumObs_long(3)     = 18
    ObsSpec%NumObs_height(3)   = 20
    ObsSpec%long_min(3)        = 10.0
    ObsSpec%long_max(3)        = 530000.0
    ObsSpec%height_min(3)      = 1.0
    ObsSpec%height_max(3)      = 12000.0
    ObsSpec%stddev(3)          = 0.0015
!  -------------------------------------
    ObsSpec%batch(4)           = 4
    ObsSpec%seconds(4)         = 1800
    ObsSpec%ob_of_what(4)      = 4          ! rp
    ObsSpec%NumObs_long(4)     = 18
    ObsSpec%NumObs_height(4)   = 20
    ObsSpec%long_min(4)        = 10.0
    ObsSpec%long_max(4)        = 530000.0
    ObsSpec%height_min(4)      = 1.0
    ObsSpec%height_max(4)      = 12000.0
    ObsSpec%stddev(4)          = 0.0015
!  -------------------------------------
    ObsSpec%batch(5)           = 5
    ObsSpec%seconds(5)         = 2400
    ObsSpec%ob_of_what(5)      = 4          ! rp
    ObsSpec%NumObs_long(5)     = 18
    ObsSpec%NumObs_height(5)   = 20
    ObsSpec%long_min(5)        = 10.0
    ObsSpec%long_max(5)        = 530000.0
    ObsSpec%height_min(5)      = 1.0
    ObsSpec%height_max(5)      = 12000.0
    ObsSpec%stddev(5)          = 0.0015
!  -------------------------------------
    ObsSpec%batch(6)           = 6
    ObsSpec%seconds(6)         = 3000
    ObsSpec%ob_of_what(6)      = 4          ! rp
    ObsSpec%NumObs_long(6)     = 18
    ObsSpec%NumObs_height(6)   = 20
    ObsSpec%long_min(6)        = 10.0
    ObsSpec%long_max(6)        = 530000.0
    ObsSpec%height_min(6)      = 1.0
    ObsSpec%height_max(6)      = 12000.0
    ObsSpec%stddev(6)          = 0.0015
!  -------------------------------------
    ObsSpec%batch(7)           = 7
    ObsSpec%seconds(7)         = 3600
    ObsSpec%ob_of_what(7)      = 4          ! rp
    ObsSpec%NumObs_long(7)     = 18
    ObsSpec%NumObs_height(7)   = 20
    ObsSpec%long_min(7)        = 10.0
    ObsSpec%long_max(7)        = 530000.0
    ObsSpec%height_min(7)      = 1.0
    ObsSpec%height_max(7)      = 12000.0
    ObsSpec%stddev(7)          = 0.0015
/
```

7. Now run the cycled data assimilation. Make directory *CycledDA_obs_rp* (in the same place as directory *Master_Calibration*) and enter this directory.

8. Copy the bash script *DAcycle001.sh* to this directory and set *EXPERIMENT* to *CycledDA_obs_rp*, *BASE_DIR* to the full path to the parent of this directory appended with */$EXPERIMENT*, *N_CYCLES* to 30, *N_OUTER_LOOPS* to 1, *N_INNER_LOOPS_MAX* to 100, *DA_WINDOW* to 3600.0, *DA_WINDOW_INT* to 3600, *OBS_NETWORK_DIR* to *$BASE_DIR/../Master_MakeBgObs_ObsNetwork*, *INITIAL_TRUTH_DIR* to *$BASE_DIR/Master_RunNLModel*, *CVT_DIR* to *$BASE_DIR/../MasterCalibration*, *CODE_DIR* to the directory containing the main fortran code, *PLOT_CODE_DIR* to the directory containing the python plotting code, *BACKGROUND_ALREADY_COMPUTED* to 0, *A* to 0.02, *B* to 0.01, *C* to 1.0E4, and *PLOT* to 1.

9. Run the back script *DAcycle001.sh*.

10. The cost function diagnostics of Fig. 9 should appear inside *$BASE_DIR/CycledDA_obs_rp/da_cycle_0007/Plots*.

10 Figure 10

The panels of Fig. 10 should also appear inside *$BASE_DIR/CycledDA_obs_rp/da_cycle_0007/Plots.* as per instructions for Fig. 9.

11 Figure 11

Much of the data shown in Fig. 11 should appear inside *$BASE_DIR/CycledDA_obs_rp/Plots* as per instructions for Fig. 9. The specific panels of Fig. 11 are made by editing *PlotMultiCycleErrors4paper.py*.

12 Figures 12 and 13

The above steps can be repeated for different options – in particular *CVT%CVT_param_opt_gb* can be set to 3 to turn-off the geostrophic balance constraint in the CVT, and *CVT%CVT_param_opt_reg* can be set to 2 to turn-off the vertical regression step that accompanies the geostrophic balance.