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.

The sample UM data mentioned in this document may be found at www.met.reading.ac.uk/~ross/downloads/Member001.nc.gz

## 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
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Α
В
                          = 0.01,
\mathbf{C}
                          = 1.0 \,\mathrm{E4}
dt
                          = 4.0,
                          = .TRUE.
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runlength
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latindex (237) latindex (238) latindex (239) latindex (240) latindex (241) latindex (242) latindex (243)	$egin{array}{l} = 246, \\ = 247, \\ = 248, \\ = 249, \\ = 250, \\ = 251, \\ = 252, \\ = 253, \end{array}$
latindex (237) latindex (238) latindex (239) latindex (240) latindex (241) latindex (242) latindex (243) latindex (244) latindex (245)	= 246, $= 247,$ $= 248,$ $= 249,$ $= 250,$ $= 251,$ $= 252,$ $= 253,$ $= 254,$ $= 255,$
latindex (237) latindex (238) latindex (239) latindex (240) latindex (241) latindex (242) latindex (243) latindex (244) latindex (245) latindex (246)	= 246, $= 247,$ $= 248,$ $= 249,$ $= 250,$ $= 251,$ $= 252,$ $= 253,$ $= 254,$ $= 255,$ $= 256,$
latindex (237) latindex (238) latindex (239) latindex (240) latindex (241) latindex (242) latindex (243) latindex (244) latindex (245) latindex (246) latindex (247)	= 246, $= 247,$ $= 248,$ $= 249,$ $= 250,$ $= 251,$ $= 252,$ $= 253,$ $= 254,$ $= 255,$ $= 256,$ $= 257,$
latindex (237) latindex (238) latindex (239) latindex (240) latindex (241) latindex (242) latindex (243) latindex (244) latindex (245) latindex (246) latindex (247)	= 246, $= 247,$ $= 248,$ $= 249,$ $= 250,$ $= 251,$ $= 252,$ $= 253,$ $= 254,$ $= 255,$ $= 256,$ $= 257,$
latindex (237) latindex (238) latindex (239) latindex (240) latindex (241) latindex (242) latindex (243) latindex (244) latindex (245) latindex (246) latindex (247) latindex (248)	$egin{array}{l} = 246, \\ = 247, \\ = 248, \\ = 249, \\ = 250, \\ = 251, \\ = 252, \\ = 253, \\ = 256, \\ = 257, \\ = 258, \end{array}$
latindex (237) latindex (238) latindex (239) latindex (240) latindex (241) latindex (242) latindex (243) latindex (244) latindex (244) latindex (246) latindex (247) latindex (248) latindex (249)	$egin{array}{l} = 246, \\ = 247, \\ = 248, \\ = 249, \\ = 250, \\ = 251, \\ = 252, \\ = 253, \\ = 254, \\ = 256, \\ = 256, \\ = 258, \\ = 259, \end{array}$
latindex (237) latindex (238) latindex (239) latindex (240) latindex (241) latindex (242) latindex (243) latindex (244) latindex (245) latindex (246) latindex (247) latindex (248)	$egin{array}{l} = 246, \\ = 247, \\ = 248, \\ = 249, \\ = 250, \\ = 251, \\ = 252, \\ = 253, \\ = 256, \\ = 257, \\ = 258, \end{array}$
latindex (237) latindex (238) latindex (239) latindex (240) latindex (241) latindex (242) latindex (243) latindex (244) latindex (245) latindex (246) latindex (247) latindex (248) latindex (249) latindex (250)	= 246, $= 247,$ $= 248,$ $= 249,$ $= 250,$ $= 251,$ $= 252,$ $= 253,$ $= 254,$ $= 255,$ $= 256,$ $= 257,$ $= 258,$ $= 259,$ $= 260,$
latindex (237) latindex (238) latindex (239) latindex (240) latindex (241) latindex (242) latindex (243) latindex (244) latindex (245) latindex (246) latindex (247) latindex (248) latindex (249) latindex (250) latindex (251)	= 246, $= 247,$ $= 248,$ $= 249,$ $= 250,$ $= 251,$ $= 252,$ $= 253,$ $= 254,$ $= 255,$ $= 256,$ $= 259,$ $= 260,$ $= 261,$
latindex (237) latindex (238) latindex (239) latindex (240) latindex (241) latindex (242) latindex (243) latindex (244) latindex (245) latindex (246) latindex (247) latindex (248) latindex (249) latindex (250) latindex (251) latindex (252)	= 246, $= 247,$ $= 248,$ $= 249,$ $= 250,$ $= 251,$ $= 252,$ $= 253,$ $= 254,$ $= 255,$ $= 256,$ $= 257,$ $= 258,$ $= 260,$ $= 261,$ $= 262,$
latindex (237) latindex (238) latindex (239) latindex (240) latindex (241) latindex (242) latindex (243) latindex (244) latindex (245) latindex (246) latindex (247) latindex (248) latindex (249) latindex (250) latindex (251)	= 246, $= 247,$ $= 248,$ $= 249,$ $= 250,$ $= 251,$ $= 252,$ $= 253,$ $= 254,$ $= 255,$ $= 256,$ $= 259,$ $= 260,$ $= 261,$

```
latindex (254)
                     = 264,
latindex (255)
                    = 265,
latindex (256)
                    = 266.
latindex (257)
                    = 267,
                     = 268,
latindex (258)
latindex (259)
                     = 269,
latindex (260)
                     = 270,
BoundSpread
                     = 100,
datadir ABCfcs
datadirCVT
                     = 'CVT. nc',
CVT file
CVT%CVT order
                     = 1,
CVT\%CVT_param_opt_ab = 2,
CVT\%CVT_param_opt_reg = 1,
CVT\%CVT vert opt sym = 1,
CVT%CVT_stddev_opt
```

- 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,
                   = 1,
NEns
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,
                  = 1,
NEnsMems
NNMC
                  = 0,
Nlats
                  = 260,
datadirRegression = '.',
datadirABCperts = '../ Master_Calibration_stage2',
datadirCVT = '...',
                  = 'CVT.nc'
{
m CVT} file
```

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
                   = 1,
NEns
                   = 1,
NEnsMems
NNMC
                   = 0,
Nlats
                   = 260,
                      '... / Master_Calibration_stage2',
datadirABCperts
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  $Master\_Calibration/Master\_Calibration\_stage2$  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,
                    = 260,
Nlats
                    = '... | Master Calibration stage2',
datadirABCperts
                       "... / Master_Calibration_stage4",
datadirConParams
datadirCVT
{
m 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.

# f 4 Figure f 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.

#### 

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

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  $Master\_Linear\_Analysis/VerticalModeCharacteristics.dat$  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
                             = '../Master_Calibration',
  datadirCVT
  {
m CVT} file
                             = 'CVT. nc',
                             = '... / Master Calibration / Master Calibration stage1',
  datadir ABCfcs
  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
                             = '... / Master_Calibration / Master_Calibration_stage2'
  datadirABCperts
  Nens
  NensMems
                             = 1
                             = 260
  Nlats
  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
  datadirUM
                             = '/home/data/UMdir'
  init um file
                             = 'Member0001 . nc'
  datadirABC out
  init ABC file
                             = 'ABC InitialConds.nc'
  latitude
  Regular_vert_grid
                             = .TRUE.
  Adv tracer
                             = .TRUE.
  gravity_wave_switch
                             = . FALSE.
  f
                             = 1.0E-4
  A
                             = 0.02
  В
                             = 0.01
  C
                             = 1.0 E4
  BoundSpread
                             = 100.
  press_source_x
                             = 200
                             = 6
  press_source_z
                             = 0.005
  {\tt press\_amp}
                             = 120
  x_scale
                             = 14
  z_scale
```

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'
                             = 'ABC Diagnostics.dat'
  diagnostics_file
                             = 7200.0
  runlength
  ndumps
                              = 4.0
  Lengthscale diagnostics
                             = . FALSE.
                              = 0.02
  В
                              = 0.01
  \mathbf{C}
                              = 1.0 E4
  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%year 0
                             = 2010
  ObsSpec%month0
                             = 1
  ObsSpec%day0
                             = 1
  ObsSpec%hour0
                             = 0
  ObsSpec%min0
                             = 0
  ObsSpec%sec0
                             = 0
  ObsSpec%NumBatches
                             = 7
  datadir_ObsSpec
                             = \ \ 'ObsSpec.dat'
  ObsSpec_file
  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
                           = 1200
ObsSpec\%seconds(3)
                                      ! rp
ObsSpec%ob of what (3)
                           = 4
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
                           = 12000.0
ObsSpec%height max (5)
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)
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.