ECCO v4 development notes

Gaël Forget Department of Earth, Atmospheric and Planetary Sciences Massachusetts Institute of Technology

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abstract

These notes pertain to the ECCO v4 state estimate, model setup, and associated codes (Forget et al., 2015). Section 1 points to the other elements of documentation that are available online, and associated download procedures. Section 2 provides guidance to ECCO v4 users interested in operating the ECCO v4 model set-up and/or reproducing the ECCO v4 solution. Section 3 documents the re-implemented estimation modules of MITgcm. Some of the included material in section 3 is expected to eventually move to the MITgcm manual.

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References

Forget, G., J.-M. Campin, P. Heimbach, C. N. Hill, R. M. Ponte, and C. Wunsch, 2015: Ecco version 4: an integrated framework for non-linear inverse modeling and global ocean state estimation. *Geoscientific Model Development Discussions*, 8 (5), 3653–3743, doi:10.5194/ gmdd-8-3653-2015, URL http://www.geosci-model-dev-discuss.net/8/3653/2015/.

1 1 downloads

² This section documents locations and directions to download the MITgcm (section 1.1), the

³ ECCO v4 model setup (section 1.2), the ECCO v4 state estimate output (section 1.3), and ⁴ related diagnostic matlab tools (section 1.4).

5 1.1 MITgcm

⁶ To install the MITgcm:

- Go to the MITgcm web-page @ mitgcm.org
- Install MITgcm using cvs as explained @ cvs
- Run MITgcm using testreport as explained @ manual, howto

¹⁰ Pre-requisites are cvs, gcc, gfortran (or alternatives), and mpi (only for parallel runs). For ¹¹ example, my laptop setup, including mpi and netcdf, involved the following mac ports:

- cvs @1.11.23_1 (active)
- wget @1.14_5+ssl (active)
- gcc48 @4.8.2_0 (active)
- mpich-default $@3.0.4_9+gcc48$ (active)
- mpich-gcc48 @3.0.4_9+fortran (active)
- netcdf $@4.3.0_2$ +dap+netcdf4 (active)
- netcdf-fortran $@4.2_{10}+gcc48$ (active)
- ¹⁹ Overridding the default mac gcc and mpich with the above requires:
- sudo port select -set gcc mp-gcc48
- sudo port select –set mpich mpich-gcc48-fortran
- ²² Using mpi and netcdf within MITgcm requires two environment variables:
- export MPI_INC_DIR=/opt/local/include
- export NETCDF_ROOT=/opt/local

²⁵ 1.2 ECCO v4 setup

Any MITgcm user can easily install the ECCO v4 setups using the setup_these_exps.csh shell script as explained @ README. It downloads global_oce_cs32/ (small setup), global_oce_llc90/ (bigger setup) and model inputs from global_oce_input_fields.tar.gz to a subdirectory called global_oce_tmp_download/. The user then wants to move its contents to MITgcm/verification/ (as shown in Fig.1) in order to allow for automated execution of the short benchmark runs via testreport using genmake2 (see section 2.1). Pre-requisites: having downloaded MITgcm (section 1.1) and mpi libraries (only if user wants to run the bigger global_oce_llc90/). The short benchmarks are ran on a daily basis to ensure continued compatibility with the

The short benchmarks are ran on a daily basis to ensure continued compatibility with the up to date MITgcm. While the short benchmarks only go for a few time steps, global_oce_llc90/

 $_{35}$ also is the basic setup that produces the 1992-2011 ECCO v4 ocean state estimate (Forget et al.,

³⁶ 2015) when configured accordingly (as explained in section 2.2). Thus running the short bench-

³⁷ marks (section 2.1) is a useful step towards re-producing the state estimate (section 2.2). It

³⁸ should also be noted that an adjoint version of the short benchmarks also exist that can readily

³⁹ be run by users who access to the TAF compiler.

Figure 1: MITgcm directory structure downloaded using cvs. The ECCO v4 directories indicated with "+" were downloaded separately using setup_these_exps.csh script and moved to MITgcm/verification/.

40 1.3 ECCO v4 solution

⁴¹ The state estimate output for ECCO v4-release 1 is available via this server which is linked to

42 ecco-group.org. The various subdirectories contain monthly fields, this documentation of the solution,

⁴³ in situ and model profiles, the grid specifications and ancillary data as explained in README.docx.

⁴⁴ For example a file (or a subdirectory) can be downloaded at the command line e.g. per

45 wget --recursive ftp://mit.ecco-group.org/ecco_for_las/version_4/release1/README.docx

46 1.4 Diagnostic Tools

To help ECCO v4 and MITgcm users analyze model output obtained either per section 1.3 or per section 2.2, two sets of Matlab tools are made freely available:

• download gcmfaces and MITprof using shell script (or see getting_started.m)

• download MITgcm/utils using cvs (basic functionalities only).

Any user can for example regenerate this documentation of the solution (the gcmfaces 'standard analysis') from the section 1.3 or section 2.2 output (expectedly organized according to Fig.2) simply by executing diags_driver.m¹ and diags_driver_tex.m² in the following sequence :

```
54 dirModel='release1_20150603_c651/';
```

- 55 dirMat='release1_20150603_c651/mat/';
- 56 dirTex='release1_20150603_c651/tex/';
- 57 nameTex='standardAnalysis';
- 58 %
- ⁵⁹ diags_driver(dirModel,dirMat,1992:2011);%requires gcmfaces and MITprof in path
- 60 diags_driver_tex(dirMat,{},dirTex,nameTex);%further requires m_map in path

¹This involves MITprof that also gets installed by shell script

²User needs to install m_map for mapping and plotting.

Figure 2: Directory structure as expected by gcmfaces and MITprof toolboxes. The toolboxes themselves can be relocated anywhere as long as their locations are included in the matlab path. Advanced analysis using diags_driver.m and diags_driver_tex.m will respectively generate the mat/ directory (for intermediate computational results) and the tex/ directory (for standard analysis). This diagnostic process relies on the depicted organization of GRID/ and solution/ for automation (user will otherwise be prompted to enter directory names) and depends on downloaded copies of fields to nctiles/ (local subdirectory).

```
gcmfaces/ (matlab toolbox)
 _sample_input/ (binary files)
 __ @gcmfaces/ (matlab codes)
 __gcmfaces_calc/ (matlab codes)
 . . .
MITprof/ (matlab toolbox)
 _profiles_samples/ (netcdf files)
  _profiles_process_main_v2/ (matlab codes)
  _profiles_stats/ (matlab codes)
   . . .
GRID/ (binary output)
release 1 solution/
_____diags/ (binary output)
 __nctiles/ (netcdf output)
 __MITprof/ (netcdf output)
 __mat/ (created by gcmfaces)
___tex/ (created by gcmfaces)
other solution/
 _diags/ (binary output)
 _ . . .
. . .
```

61 2 MITgcm runs

The following procedures, commands and submission scripts allow runs of the ECCO v4 MITgcm setup – either in short regression tests (section 2.1) or for multi-decadal simulations such as the full 20 year state estimate (section 2.2). Pre-requisite for sections 2.1 and 2.2: having downloaded the MITgcm (section 1.1) and the ECCO v4 setups (section 1.2). Pre-requisite for section 2.2: having downloaded forcing fields and a few other binary model inputs (listed below).

67 2.1 regression tests

Short benchmarks of the MITgcm and ECCO v4 setup are run using testreport command line
utility (see Fig.2; howto). Serial runs are executed simply at the command line e.g. per

```
70 ./testreport -t global_oce_cs32
```

71 OT

```
72 ./testreport -skipdir global_oce_llc90
```

The reader is referred to 'testreport –help' and how to for additional explanation about such 73 commands. If everything proceeds as expected then the result of the comparison with the 74 reference result is reported to screen as shown in abbreviated form in Fig. 3. Depending on 75 your machine environment the agreement with the reference result may be lower in which case 76 'testreport' may indicate 'FAIL' (e.g. see README). Despite the dramatic character of such 77 message, this is generally ok and does not prevent reproducing full model solutions accurately 78 (see section 2.2). If the testreport process gets interrupted then it is often safer to clean up 79 experiment directories (e.g., by executing ./testreport -clean -t global_oce_*) and start over. 80

```
----T-----
default 10
                          ----S-
GDM
          с
                    m
                       s
                                 m
                                    s
 раR
          g
                    е
                          m
             m
                m
                       .
                              m
                                 е
nnku
          2
             i
                       d
                          i
                а
                              a
                                 а
                                    d
                    а
          d
2 d e
      n
             n
                х
                    n
                          n
                              x
                                 n
Y Y Y Y>14<16 16 16 16 16 16 16 16 16
                                        pass
                                             global_oce_cs32
```

Figure 3: Abbreviated output of testreport to screen.

The above 'testreport' commands deserve a couple more specific comments. The first com-81 mand runs the global_oce_cs32/ benchmark solely. The second command will run all MITgcm 82 benchmarks including global_oce_cs32/ but not the global_oce_llc90/ benchmark that requires 83 at least 12 processors in forward (96 in adjoint) and therefore should not be run in serial mode 84 (doing so may crash your laptop). It is thus excluded by using the 'skipdir' option. It should 85 be stressed however that $global_oce_cs32/$ depends on the files in $global_oce_llc90/$ (which is the 86 main setup) rather than duplicating them. Therefore global_oce_llc90/ must not be removed 87 from MITgcm/verification for global_oce_cs32/ to work. 88

⁸⁹ Running the short benchmarks with mpi (assuming it has been installed) is equally simple:

```
90 ./testreport -of ../tools/build_options/linux_amd64_ifort+mpi_ice_nas \
91 -j 4 -MPI 96 -command 'mpiexec -np TR_NPROC ./mitgcmuv' \
92 -t global_oce_llc90
```

⁹³ for example will run the forward global_oce_llc90/ benchmark on 96 processors using an ifort ⁹⁴ compiler. Note that the specifics (number of processors and compiler choice) are to be deter-⁹⁵ mined by the user and are machine dependent.

Often in massively parallel computing environments, it is common that mpi jobs can only be run within a queuing system. The submission script in Fig.4 (that is also machine specific) provides an example on how to do it. It contains 3 hard-coded switches : fwdORad = 1 (2 for adjoint); numExp = 1 (2 for llc90); excludeMpi = 0 (1 for serial). This script should be located and submitted from MITgcm/verification. It is also common that compute nodes cannot access certain compilers, in which case the user may want to proceed in two steps:

102 1. compile outside of the queuing system using e.g. per

```
./testreport -of ../tools/build_options/linux_amd64_ifort+mpi_ice_nas \
-j 4 -MPI 96 -command 'mpiexec -np TR_NPROC ./mitgcmuv' \
-t global_oce_llc90 -norun
```

2. submit the Fig.4 script, after adding -q to the 'opt' variable to skip compilation.

Running adjoint benchmarks requires access to the TAF compiler. The calls to testreport 107 (see above) then only need to be slightly altered by appending the '-ad' option (for either 108 serial or mpi jobs) and replacing 'mitgcmuv' with 'mitgcmuv_ad' (only for mpi jobs). It should 109 also be noted that, unlike other MITgcm benchmarks, global_oce_cs32/ and global_oce_llc90/ 110 do not include any adjoint specific 'code_ad/' directory as they simply use the forward model 111 'code/' directory instead. Since testreport relies on the existence of 'code_ad/' for its adjoint 112 option though, it is necessary to soft link 'code/' to 'code_ad/' in both global_oce_cs32/ and 113 global_oce_llc90/ accordingly in order to to run their 'testreport -ad' versions. 114

Figure 4: Example script to run mpi testreport via a queueing system (machine dependent).

```
#PBS -S /bin/csh
#PBS -1 select=1:ncpus=16:model=ivy+4:ncpus=20:model=ivy
#PBS -1 walltime=02:00:00
#PBS -q devel
#PBS -m n
#environment variables and libraries
limit stacksize unlimited
module purge
module load modules comp-intel/2013.1.117 mpi-sgi/mpt.2.10r6 netcdf/4.0
#
setenv LD_LIBRARY_PATH ${LD_LIBRARY_PATH}:${HOME}/lib
setenv MPI_IB_TIMEOUT 20
setenv MPI_IB_RAILS 2
setenv MPI_IB_FAILOVER 1
setenv MPI_CONNECTIONS_THRESHOLD 2049
#local variables and commands
#-----
set fwdORad = 1
set numExp = 1
set excludeMpi = 0
#
if ( \{numExp\} == 1\} then
 set nameExp = global_oce_cs32
 set NBproc = 6
else
 set nameExp = global_oce_llc90
 set NBproc = 96
endif
#
if ( ${excludeMpi} == 1 ) then
 set opt = '-of ../tools/build_options/linux_amd64_ifort -j 4'
else
 set opt = '-of .../tools/build_options/linux_amd64_ifort+mpi_ice_nas -j 4'
endif
#
if ( ${fwdORad} == 1 && ${excludeMpi} == 0 ) then
  ./testreport ${opt} -MPI \
  ${NBproc} -command 'mpiexec -np TR_NPROC ./mitgcmuv' -t ${nameExp}
else if ( fwdORad == 2 && fexcludeMpi == 0 ) then
 ./testreport ${opt} -MPI \
 ${NBproc} -command 'mpiexec -np TR_NPROC ./mitgcmuv_ad' -ad -t ${nameExp}
else if ( ${fwdORad} == 1 && ${excludeMpi} == 1 ) then
  ./testreport ${opt} -t ${nameExp}
else if ( ${fwdORad} == 2 && ${excludeMpi} == 1 ) then
  ./testreport ${opt} -ad -t ${nameExp}
endif
exit
                                        9
```

115 2.2 full ECCO v4 runs

The 1992-2011 ECCO v4 ocean state estimate (Forget et al., 2015) is reproduced on a monhtly basis to ensure continued compatibility with the up to date MITgcm. Re-running the baseline 20 year solution (or any other 20 year of global_oce_llc90/) on 96 processors may take about 8 to 12 hours (depending on the computing environment). Unlike for the short benchmarks of section 2.1, in the case of these longer model runs:

- the model is compiled and run outside of testreport.
- the model is compiled with compiler optimization.
- additional forcing and binary input is necessary.
- additional memory and/or disk space is necessary.

The reader is referred to how for a general explanation of such practice. The typical compi-125 lation sequence for the ECCO v4 forward model (i.e. the model setup in global_oce_llc90/) is 126 shown in Fig.5. The tamc.h_itXX and profiles.h_itXX headers (see Fig.5) allow for additional 127 time steps and in situ profiles input, respectively. Once done with compilation, the user typi-128 cally creates and enters a run directory, links the model executable and inputs into place (see 129 Fig.6), and submits a job to the queueing system (see Fig.7). User interested in obtaining the 130 additional model input required to reproduce the baseline 1992-2011 solution (i.e. the ECCO 131 v4 state estimate) are advised to contact ecco-support@mit.edu. This model input consists of: 132

- the forcing files (EIG*199? EIG*20??).
- the initial conditions (pickup^{*}) and control vector adjustsments (xx_^{*}).
- the insitu data sets inputs (*feb2013*.nc) used for benchmarking purposes (see below).

Once the model run has completed, one wants to verify that it accurately reproduces the 136 reference result – or detect that a mistake was made. To this end, a mechanism that is analogous 137 to testreport but is geared towards benchmarking long runs was introduced by Forget et al. 138 (2015). It is operated by testreport_ecco.m within Matlab. The pre-requisite is to add the 139 reference result directory 'MITgcm/verification/global_oce_llc90/results_itXX/' to the Matlab 140 path. As explained in Forget et al. (2015) testreport_ecco.m compares time series of global 141 mean variables, and other characteristics of the solution, to the reference state estimate values. 142 The array of tests can be extended to e.g. meridional transports by adding gcmfaces to the 143 Matlab path. The typical call sequence is indicated in the help of testreport_ecco.m and in 144 Fig.8 that also illustrates the typical display of the benchmarking results report to the user 145 screen. The expected level of accuracy for re-runs of the baseline 20 year solution (with an up 146 to date MITgcm code on any given computer) is reached when the displayed values are < -4147 (see Forget et al., 2015, for details). In cases when some of the tests were omitted (e.g. because 148 gcmfaces was not in the Matlab path) the display will show NaN for omitted tests. From the 149 generated model output, one may further easily compute and display many diagnostic quantities 150 using the gcmfaces standard analysis for example (see section 1.4). 151

Figure 5: Compilation directives, outside testreport, for intensive model runs. On a different machine (computer) another build option file such as linux_amd64_gfortran or linux_amd64_ifort11 should be used. To compile the adjoint, users need a TAF license and to replace 'make -j 4' with 'make adall -j 4'. Note : the '-mods=../code' specification can be omitted if the build directory contains the 'genmake_local' file).

```
cd verification/global_oce_llc90/build
../../../tools/genmake2 -optfile=\\
../../tools/build_options/linux_amd64_ifort+mpi_ice_nas -mpi -mods=../code
make depend
\rm tamc.h profiles.h
cp ../code/tamc.h_itXX tamc.h
cp ../code/profiles.h_itXX profiles.h
make -j 4
```

Figure 6: Example script to setup the 20 year ECCO v4 state estimate. It is implied that user has filled directories /bla, /blaa, /blaaa and /blaaa with appropriate forcing, observational, control vector, and pickup files.

```
#!/bin/csh -f
set forcingDir = ~/bla
                = ~/blaa
set obsDir
set ctrlDir
                = ~/blaaa
                = ~/blaaaa
set pickDir
source ../input_itXX/prepare_run
cp ../build/mitgcmuv .
\rm pick*ta EIG*
ln -s ${forcingDir}/EIG* .
ln -s ${obsDir}/* .
ln -s ${ctrlDir}/xx* .
ln -s ${pickDir}/pick* .
exit
```

Figure 7: Example script to run the 20 year ECCO v4 state estimate on 96 processors (machine dependent).

```
PBS -S /bin/csh
#PBS -1 select=1:ncpus=16:model=ivy+4:ncpus=20:model=ivy
#PBS -1 walltime=12:00:00
#PBS -q long
#environment variables and libraries
limit stacksize unlimited
module purge
module load modules comp-intel/2013.1.117 mpi-sgi/mpt.2.10r6 netcdf/4.0
#
setenv LD_LIBRARY_PATH ${LD_LIBRARY_PATH}:${HOME}/lib
setenv MPI_IB_TIMEOUT 20
setenv MPI_IB_RAILS 2
setenv MPI_IB_FAILOVER 1
setenv MPI_CONNECTIONS_THRESHOLD 2049
#run MITgcm
#-----
mpiexec -np 96 dplace -s1 ./mitgcmuv
exit
```

Figure 8: Calling sequence to be executed form within matlab to verify that their re-run of the 20 year ECO v4 state estimate is acceptably close to the released state estimate.

¹⁵² 3 re-implemented ecco and ctrl packages

153 State estimation consists in minimizing a least squares distance, J(u), that is defined as

$$\mathbf{J}(\mathbf{\mathfrak{u}}) = \sum_{i} \alpha_{i} \times (\mathbf{d}_{i}^{T} \mathbf{R}_{i}^{-1} \mathbf{d}_{i}) + \sum_{j} \beta_{j} \times (\mathbf{\mathfrak{u}}_{j}^{T} \mathbf{\mathfrak{u}}_{j})$$
(1)

$$\mathbf{d}_i = \mathcal{P}(\mathbf{m}_i - \mathbf{o}_i) \tag{2}$$

$$\mathbf{m}_i = \mathcal{SDM}(\mathbf{v}) \tag{3}$$

$$\mathfrak{v} = \mathcal{Q}(\mathfrak{u}) \tag{4}$$

$$\mathfrak{u} = \mathcal{R}(\mathfrak{u}') \tag{5}$$

where d_i denotes a set of model-data differences, α_i the corresponding multiplier, $\mathbf{R_i}^{-1}$ the

corresponding weights, \mathfrak{u}_j a set of non-dimensional controls, β_j the corresponding multiplier,

and additional symbols appearing in Eqs. 2-5 are defined below. The implementation of Eqs.1-5

¹⁵⁷ and the adjoint interface within the MITgcm is charted in Fig. 9. A general presentation of

Eqs. 1-5 and Fig. 9 can be found in Forget et al. (2015). The focus here is on the underlying code

development in 'pkg/ecco' and 'pkg/ctrl' of MITgcm. These features are now tested daily via

 $_{160}$ global_oce_cs32/ (adjoint experiment) that will also serve here for illustration in this document.



Figure 9: Chart of the organization and roles of MITgcm estimation modules. Additional details are reported in the MITgcm manual, Forget et al. (2015), and section 3 of this document.

¹⁶¹ 3.1 pkg/ecco run-time parameters and algorithm

Model counterparts (m_i) to observational data (o_i) derive from adjustable model parameters (\mathfrak{v}) 162 ; see section 3.2) through the model dynamics (\mathcal{M} ; see Forget et al. 2015), diagnostic computa-163 tions (\mathcal{D}) , and averaging (or subsampling in 'pkg/profiles') in space and time (\mathcal{S}) . The physical 164 variable in m_i is specified at run time via the first characters in 'gencost_barfile' (to match the 165 observed variable in o_i) as illustrated in this data.ecco and that data.ecco. The list of imple-166 mented variables as of the MITgcm checkpoint c65l consists of 'm_eta', 'm_sst', 'm_sss', 'm_bp', 167 'm_tauZon', 'm_tauMer', 'm_theta', 'm_salt'³. In the case of three dimensional variables (e.g. 168 'm_theta' or 'm_salt') the 'gencost_is3d' run-time option must be set to .TRUE. in data.ecco (it 169 is .FALSE. by default). In cases when two different averages of the same variable may be needed 170 (e.g. daily and monthly) then a suffix starting with '_' can be added (such as '_day' and '_mon'). 171 The file name for the observational fields (o_i) and the model-data uncertainty field $(\sqrt{\mathbf{R}_i})$ are 172 specified at run time via 'gencost_datafile'⁴ and 'gencost_errfile'⁵ respectively. The cost function 173 multiplier (α_i) further needs to be specified by 'mult_gencost' (it is 0. by default). 174

Both \mathcal{D} and \mathcal{S} in Eq.3 are mainly carried out as the forward model steps through time, 175 respectively by ecco_phys.F and cost_averages generic.F, and m_i is written to file periodically. 176 m_i and o_i normally are time series of daily or monthly averages⁶, as specified at run time via 177 'gencost_avgperiod'. However dense time series of model time steps can also be employed for 178 testing purposes as illustrated in this data.ecco. Furthermore climatologies of m_i can be formed 179 from its time series by $cost_genread$. F to allow for comparison with observational o_i climatologies. 180 This part of the m_i processing is carried out within cost_generic.F (see below) after the full time 181 series has been written to file. It is activated via a 'gencost_preproc' option as illustrated in 182 this data.ecco. 183

Model-data misfits are computed (Eq. 2) upon completion of the forward model simulation 184 by cost_generic.F that relies on ecco_toolbox.F for elementary operations and on cost_genread.F 185 for re-reading m_i from file. Plain model-data misfits $(m_i - o_i)$ can be penalized directly (i.e. 186 used in Eq. 1 in place of d_i). More generally though misfits to be penalized (d_i in Eq. 1) derive 187 from $m_i - o_i$ through a generic post-processor (\mathcal{P} in Eq. 2). They can thus be smoothed in 188 space at run time via 'gencost_posproc' for example (see this data.ecco). The overall sequence 189 of operations for one cost function term is charted in Fig.10. The distinction between 'preproc' 190 and 'posproc' matches that between Eqs. 3 and 2. Most concretely the pre-processing ends and 191 post-processing starts at the computation of $m_i - o_i$ using 'ecco_diffmsk' in cost_generic.F. 192

³!!! pending modification ... right now : 'eta', 'sst', 'sss', 'bp', 'tauZon', 'tauMer', 'theta', 'salt'

⁴The observational field time series may be split in yearly files finishing in e.g. '_1992', '_1993', etc.

⁵The option for time varying error fields remains to be implemented in gencost.

⁶In principle any frequency should be possible but only 'month', 'day', and 'step' are currently implemented.

Algorithm 1 Generic cost function algorithm.			
\triangleright Argument list defines the cost function			
\triangleright Initialize local array to 0			
\triangleright Copy mask to local array			
\triangleright Loop over time steps, days or months			
\triangleright Get file names, pointers			
\triangleright Read, process model field			
\triangleright Read one record			
\triangleright Average records			
\triangleright Read observational field			
\triangleright Compute masked model-data misfit			
\triangleright Smooth masked misfit			
\triangleright Add to cost function			
20: end function			

Figure 10: Chart of the generic cost function routine in pkg/ecco.

¹⁹³ 3.2 pkg/ctrl run-time parameters and algorithm

The control problem is non-dimensional by default, as reflected by the omission of weights 194 in control penalties $(\mathfrak{u}_j^T\mathfrak{u}_j, \text{Eq.1})$. Three basic options are implemented: time variable two 195 dimensional controls ('gentim2d'), time-invariant 2D controls ('genarr2d'), and time-invariant 196 3D controls ('genarr3d'). In all three, non-dimensional controls (\mathfrak{u}_i) are scaled to physical units 197 (\mathfrak{v}_i) through multiplication by their respective uncertainty fields, as part of the generic pre-198 processor Q (Eq.4). For any adjustable parameter that is activated at run-time (by setting 199 'xx_gentim2d_file' in data.ctrl) the corresponding uncertainties must be provided in the form of 200 weights (by setting 'xx_gentim2d_weight' in data.ctrl). Before discussing these specifications in 201 more detail, it should be stressed that if any uncertain parameter is activated but the weight 202 is not specified (or vice versa) then pkg/ctrl signals the inconsistency and then stops the model 203 during its initialization (since nothing would not get adjusted otherwise). 204

An adjustable model parameter u_i gets activated at run time according to the first characters 205 in 'xx_gentim2d_file' (or the 'genarr2d' or 'genarr3d' versions) as illustrated in this data.ctrl 206 and that data.ctrl. In the case when several adjustments are sought in one model parameter 207 (e.g. time mean and time variable forcing adjustments treated separetely) then a suffix starting 208 with '_' can be added to the 'xx_gentim2d_file' specification (such as '_mean' and '_anom'; see 209 this data.ctrl). Each weight binary file (specified via 'xx_gentim2d_weight') must contain at least 210 one map of $\frac{1}{\sigma^2}$ where σ_u is the corresponding uncertainty map that will be used to scale \mathfrak{u}_j to 211 physical units (as part of Q in Eq.4).⁷ Time variable weights can also be provided by specifying 212 'variaweight' as a pre-processing option in data.ctrl ('xx_gentim2d_preproc'; further discussed 213 below). 214

Besides the scaling to physical units, the generic pre-processor Q can include the spa-215 tial correlation model and/or a mapping in time such as the cyclic repetition of mean sea-216 sonal controls for example. Such pre-processing options are set per 'xx_gentim2d_preproc' 217 run-time parameters. Refined specifications are needed in some cases, which can be done 218 via 'xx_gentim2d_preproc_i' (integer), 'xx_gentim2d_preproc_r' (real), 'xx_gentim2d_preproc_c' 219 (character string). In the case of time-variable adjustable model parameters, the frequency is 220 specificied per 'xx_gentim2d_period' and the multiplier for the cost function penalty (β_i in Eq. 221 1) is specified per 'mult_gentim2d' (which is 0. by default). In the case of time-invariant 3D 222 model parameters, bounds can further be specified via the 'xx_genarr3d_bounds' run-time pa-223 rameter.⁸ The pre-conditioner \mathcal{R} (in Eq. 5) does not appear in the estimation problem itself 224 (Eq.1), as it only serves to push an optimization process preferentially towards certain directions 225 of the control space. It is specified via the 'gentim2dPrecond' (or the 'genarr2d' or 'genarr3d' 226 versions) run-time parameter (which is 1. by default). 227

In the implementation of Eqs. 4 and 5, generality and versatility is greatly improved by operating virtually all of the pre-processing at initialization time. This is done by ctrl_map_ini_genarr.F ('genarr2d', 'genarr3d') and ctrl_map_ini_gentim2d.F ('gentim2d'). By the end of the processing steps, the effective version of the parameter adjustments ('gentim2d', 'genarr2d') or of the adjusted model parameters ('genarr3d') are written to disk (with '.effective' in the file name). Time-invariant model parameters are set during model initialization, so their potential adjustments are generally also made before the model time-stepping starts ('genarr2d', 'genarr3d').

⁷Eventually options should be added to specify an uncertainty field or constant instead

⁸In principle this should be possible also for 'genarr2d' and 'gentim2d' but this is not yet implemented.

Forcing variables are however reset at each time-step, so their potential adjustment via 'gen-235 tim2d' are made during the model run. In this case it should be noted that the effective version 236 always consists of a full time series, whether it contains e.g. repeated seasonal mean adjustments 237 or series of interannual anomalies. This choice allows for a uniform, simple and general treatment 238 of all varieties of time-variable parameter adjustments needed during the model integration (the 239 temporal interpolation carried out in ctrl_map_gentim2d.F). This approach is particularly ad-240 vantageous in the context of the checkpointed adjoint model development, and generally implies 241 a marginal overhead in disk storage as compared with e.g the adjoint checkpoints (see MITgcm 242 manual) or the forcing fields thermselves. The cost function that is commonly included to pe-243 nalize parameter adjustments ($\mathfrak{u}_i^T\mathfrak{u}_i$, Eq.1) is itself computed once the model run has completed, 244 along with the other cost function terms (section 3.1). 245

²⁴⁶ 3.3 Compiling options for pkg/ecco, pkg/ctrl, etc.

Much of the legacy code that has been distributed as part of 'pkg/ecco' and 'pkg/ctrl' in the past is now deprecated – it is superseeded by the generic cost function and control codes presented above. Most of the deprecated codes had not been tested or maintained for many years, and consist of variations of the same operations duplicated many times. Another issue was the lack of organization amongst the deprecated codes (unlike in Fig.9). The consensus was that there was no point in keeping them around much longer.

For the time being the deprecated codes still exist but they are not compiled anymore unless the 'ECCO_CTRL_DEPRECATED' compile option is added in e.g. 'ECCO_CPPOPTIONS.h' (see below for details). To further facilitate the transition from old to new setup, the ctrlUseGen run-time parameter allows a switch between the old and new (generic) treatment of control vectors (assuming that 'ECCO_CTRL_DEPRECATED' was defined at compile time). As a side note: there is one non-generic feature that ISN'T deprecated since it has not been re-implemented in generic fashion, which is the control of open boundary conditions.

The deprecation of the legacy codes leads to a vast reduction in the volume of estimation 260 codes (30% of the code treated by automatic differentiation, which includes the entire phys-261 ical model, was removed in the process), a vast addition of capabilities (new or pre-existing 262 functionalities are now available for any gridded data set), and a greatly improved flexibility 263 (virtually all options can now be switched on/off at run time). Furthermore, the ecco, ctrl and 264 autodiff packages were made independent of each other, and to follow common MITgcm coding 265 practices. For example they can now be switched on/off at run time, independently (by virtue 266 of useECCO, useCTRL, useAUTODIFF). 267

Compiling options are typically found in the 'code/' directory of any given setup of MITgcm (when customized) or in the corresponding MITgcm package (when using defaults). The most obvious difference between the new setup and an old setup is that CPP_OPTIONS.h now disregards ECCO_CPPOPTIONS.h and uses the following instead :

- AUTODIFF_OPTIONS.h contains the few compile directives of pkg/autodiff. The maximum numbers of time steps are set in tamc.h
- ECCO_OPTIONS.h contains compile directives of pkg/ecco. Very few remain necessary, since all generic cost function settings can now be chosen at run time. The maximum numbers of cost terms are set in ecco.h

- CTRL_OPTIONS.h contains compile directives of pkg/ctrl. Very few remain necessary, since all generic control settings can now be chosen at run time. The maximum numbers of controls are set in CTRL_SIZE.h
- along with MOM_COMMON_OPTIONS.h, GMREDI_OPTIONS.h, GGL90_OPTIONS.h,
 PROFILES_OPTIONS.h, EXF_OPTIONS.h, SEAICE_OPTIONS.h, DIAG_OPTIONS.h