Instructions for reproducing ECCO Version 4 Release 4

Ou Wang and Ian Fenty

NASA Jet Propulsion Laboratory/California Institute of Technology

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1. Introduction

These instructions describe how to reproduce the ECCO Version 4, Release 4 (V4r4) ocean and sea-ice state estimate (ECCO Consortium, et al., 2021) and the unoptimized, "iteration 0" model simulation.

Daily and monthly-mean fields of the V4r4 state estimate are available from NASA's Physical Oceanography Distributed Active Archive Center (PO.DAAC), <u>https://podaac.jpl.nasa.gov/ECCO</u>. Instructions for downloading the solution from PO.DAAC can be found on the ECCO website, <u>https://ecco-group.org/products-ECCO-V4r4.htm</u>.

The document is organized as follows. Section 2 describes how to obtain the core source code of the <u>MIT general circulation model</u> (MITgcm). Section 3 describes how to download the source code and the model configuration files that are specific to the V4r4 solution. Section 4 deals with downloading the model's atmospheric forcing, initial conditions, and other needed files. In section 5, we show how to compile and run the model. Section 6 explains how to stop and restart the simulation. Section 7 describes how to customize which fields are saved during the model simulation. Finally, Section 8 provides instructions for reproducing the unoptimized, "iteration 0" model simulation.

2. Downloading the MITgcm source code

The ECCO V4r4 state estimate is a free-running solution of the MIT general circulation model. Reproducing the state estimate requires compiling and running the model source code version *checkpoint 66g,* which is the same code version used to produce the solution.

Warning: The MITgcm code is always evolving and therefore you must use checkpoint 66g to exactly reproduce the solution.

The MITgcm source code *checkpoint 66g* is available from the MITgcm GitHub repository. Begin by first creating a working directory, here labelled **WORKINGDIR**. All directories and files downloaded hereafter will be inside your **WORKINGDIR**.

mkdir WORKINGDIR cd WORKINGDIR

Clone the MITgcm *checkpoint66g* repository using *git*. The *git clone* command will create a subdirectory called **MITgcm**.

git clone <u>https://github.com/MITgcm/MITgcm.git</u> -b checkpoint66g

Alternatively, you can download the MITgcm source code using *wget* (or equivalent), unzip, and rename as follows:

```
wget https://github.com/MITgcm/MITgcm/archive/refs/tags/checkpoint66g.zip
unzip checkpoint66g.zip
mv MITgcm-checkpoint66g MITgcm
```

Your directory structure should now look like this:

```
WORKINGDIR
└── MITgcm
```

3. Downloading specific code and run-time parameters

In addition to the core MITgcm *checkpoint* 66g code, some additional MITgcm code files and the model's run-time parameter files (also referred to as "**namelist**" files) are needed. These files are available from the ECCO-GROUP GitHub repository:

https://github.com/ECCO-GROUP/ECCO-v4-Configurations/tree/master/ECC0v4%20Release%204

From WORKINGDIR, clone the ECCO-v4-Configurations repository, then make a directory for running the model, here labelled ECCOv4/release4. Finally, copy the code/ and namelist/ directories to the ECCOv4/release4 directory:

```
cd WORKINGDIR
git clone https://github.com/ECCO-GROUP/ECCO-v4-Configurations.git
mkdir -p ECC0V4/release4
cp -r "ECCO-v4-Configurations/ECC0v4 Release 4/code/" ECC0V4/release4/code
cp -r "ECCO-v4-Configurations/ECC0v4 Release 4/namelist/" ECC0V4/release4/namelist
```

Your directory structure should now look like this:

```
WORKINGDIR

    ECCO-v4-Configurations

    ECCOV4

    release4

    _____ code

    _____ namelist

    MITgcm
```

4. Download atmospheric forcing, initial conditions, and other input files

ECCO V4r4's atmospheric forcing, model initial conditions, and other required input files are available in a dataset, called **ECCO Ancillary Data (Version 4 Release 4)**, hosted on PO.DAAC. The ancillary dataset has 8 file archives (gzipped tarballs), 6 of which are required (see *Table 1*). Combined file size of these 6 files is approximately 200 GB. The dataset "short name" is **ECCO_L4_ANCILLARY_DATA_V4R4** and its PO.DAAC url is: https://podaac.jpl.nasa.gov/dataset/ECCO_L4_ANCILLARY_DATA_V4R4

FILENAME	DESCRIPTION
ancillary_data_doc_ECCO_V4r4.tar.gz	documentation
ancillary_data_input_init_ECCO_V4r4.tar.gz	files required to initialize the model
ancillary_data_input_forcing_ECCO_V4r4.tar.gz	atmospheric boundary conditions and other fields used to force the model
<pre>ancillary_data_native_grid_files_ECC0_V4r4.tar.gz</pre>	files defining the model grid geometry
ancillary_data_data_constraints_ECCO_V4r4.tar.gz	observational data used to constrain the model. Except for in situ data, data are mapped to the model grid as single precision flat binary format. The in-situ data are provided in NetCDF format.
ancillary_data_misc_ECCO_V4r4.tar.gz	miscellaneous files

Table 1: The 6 files from the ECCO V4r4 ancillary dataset required to reproduce the solution

An account with NASA Earthdata system is required to download these files. New Earthdata accounts can be made here: <u>https://urs.earthdata.nasa.gov/home</u>

There are several different ways to get these files. One way is to navigate to the Earthdata webpage for the dataset and simply click on each file one at a time to initiate transfers, https://cmr.earthdata.nasa.gov/virtual-directory/collections/C2096684707-

Pocloub/temporal/1992/01/01

Another way is to navigate to the "Earthdata Search" page associated with the dataset, and then click on the download icons associated with each of the 6 files: https://search.earthdata.nasa.gov/search/granules?p=C2096684707-POCL0UD

Detailed instructions for **batch** downloading these files from the command line (using *wget*) or from within a Jupyter Python notebook are provided on the ECCO-GROUP GitHub repository: https://github.com/ECC0_GROUP/ECC0_ACCESS/blob/master/PODAAC/Downloading ECC0 datasets from PODAAC/README.md

Alternatively, because there are only 6 files, you can download them one at a time using *wget* by following the instructions below. Note: replace **YOURUSERNAME** with *your* Earthdata login and use your Earthdata password when prompted.

```
cd WORKINGDIR/ECCOV4/release4
mkdir input
cd input
wget --user YOURUSERNAME --ask-password https://archive.podaac.earthdata.nasa.gov/podaac-ops-
cumulus-protected/ECC0_L4_ANCILLARY_DATA_V4R4/ancillary_data_misc_ECC0_V4r4.tar.gz
wget --user YOURUSERNAME --ask-password https://archive.podaac.earthdata.nasa.gov/podaac-ops-
cumulus-protected/ECCO L4 ANCILLARY DATA V4R4/ancillary data doc ECCO V4r4.tar.gz
wget --user YOURUSERNAME --ask-password https://archive.podaac.earthdata.nasa.gov/podaac-ops-
cumulus-
protected/ECC0_L4_ANCILLARY_DATA_V4R4/ancillary_data_native_grid_files_ECC0_V4r4.tar.gz
wget --user YOURUSERNAME --ask-password https://archive.podaac.earthdata.nasa.gov/podaac-ops-
cumulus-protected/ECC0_L4_ANCILLARY_DATA_V4R4/ancillary_data_input_forcing_ECC0_V4r4.tar.gz
wget --user YOURUSERNAME --ask-password https://archive.podaac.earthdata.nasa.gov/podaac-ops-
cumulus-protected/ECCO L4 ANCILLARY DATA V4R4/ancillary data data constraints ECCO V4r4.tar.gz
wget --user YOURUSERNAME --ask-password https://archive.podaac.earthdata.nasa.gov/podaac-ops-
cumulus-protected/ECC0_L4_ANCILLARY_DATA_V4R4/ancillary_data_input_init_ECC0_V4r4.tar.gz
```

Once you have the 6 archives, use the following command to extract the files, and delete the original archives (optional).

tar xzvf ancillary_data_misc_ECC0_V4r4.tar.gz
tar xzvf ancillary_data_doc_ECC0_V4r4.tar.gz
tar xzvf ancillary_data_native_grid_files_ECC0_V4r4.tar.gz
tar xzvf ancillary_data_input_forcing_ECC0_V4r4.tar.gz
tar xzvf ancillary_data_data_constraints_ECC0_V4r4.tar.gz
tar xzvf ancillary_data_input_init_ECC0_V4r4.tar.gz
(optional) rm ancillary_data* ECC0_V4r4.tar.gz

Your directory structure should now look like this:



5. Compile and run

The compilation and run of the model are compiler and platform specific. In this section we show how to compile and run the model on the NASA's Pleiades Supercomputer as of Jan 2022.

5.1 Compile

Before compiling the code and running the model, one has to load the required modules, including compiler and NetCDF packages, with the following commands:

```
module purge
module load comp-intel/2020.4.304
module load mpi-hpe/mpt.2.25
module load hdf4/4.2.12
module load hdf5/1.8.18_mpt
module load netcdf/4.4.1.1_mpt
```

The modules listed above are the current versions of the available modules on Pleiades as of January 14, 2022. It is generally recommended to use newer versions of modules as available.

The commands to compile are listed below. A set of system-specific "build options" are specified in WORKINGDIR/ECCOV4/release4/code/linux_amd64_ifort+mpi_ice_nas

```
cd WORKINGDIR/ECCOV4/release4
mkdir build
cd build
export ROOTDIR=../../MITgcm
../../MITgcm/tools/genmake2 -mods=../code
        -optfile=../code/linux_amd64_ifort+mpi_ice_nas -mpi
make -j16 depend
make -j16 all
cd ..
```

Note: use the full path of WORKINGDIR. If compiled successfully, the model executable will be WORKINGDIR/ECCOV4/release4/build/mitgcmuv.

Warning: Different systems require different build options! Example build option files for several platforms and compilers can be found in MITgcm/tools/build_options/ You may need to make a build options file suitable for your own system in order for the Makefile to use appropriate compiler options and to find required libraries.

The model needs NetCDF installed to read in situ profile data stored in NetCDF format. The compiler (the genmake2 command above) will check if NetCDF is correctly installed and linked, and print out a warning message (see below) if otherwise.

WARNING: the "profiles" package was enabled but tests failed to compile NetCDF applications. Please check that:

- 1) NetCDF is correctly installed for this compiler and
- the LIBS variable (within the "optfile") specifies the correct NetCDF library to link against.

Due to this failure, the "profiles" package is now DISABLED.

5.2 Run

An example of the run script for Pleiades (called pbs_eccoV4r4.csh) is included at the end of this document. The example PBS script will reproduce V4r4's 26-yr results from 1992 through 2017 in one pass (without stopping). The requested wall clock time is 24 hours (**#PBS -l** walltime=24:00:00). While 24 hours is usually sufficient to finish the 26-year model integration period on Pleiades, one may have to increase the job run time on a different machine or when increasing the amount of model diagnostic output.

To submit the job to the PBS scheduler, run the command:

qsub pbs_eccoV4r4.csh

The job may wait for some time in the queue before executing. The run directory will be created by the **pbs_eccoV4r4.csh** script (once after it is out of the queue). The name of the run directory

will be **WORKINGDIR/ECCOV4/release4/run**. To change the name of the run directory, simply modify the csh script.

After running, your directory structure should look like this:

WORKINGDIR ├── ECCO-v4-Configurations └── ECCOV4	
└── release4	
│	
│	
│	
│	
│ └── run	
└── MITgcm	

6. Stopping and restarting a run

Normally, the model simulation should be run non-stop for the entire time period. However, the simulation can be interrupted and then restarted partway through by making use of a "pickup" file. MITgcm pickup files are snapshots of the model state which can serve as model initial conditions. To learn more about how to use pickup files in the MITgcm, see: https://mitgcm.readthedocs.io/en/latest/getting_started/getting_started.html?highlight=pickup p#restart-pickup-files

The normal ECCO model simulation starts from a pickup file corresponding with time step 1: WORKINGDIR/ECCOV4/release4/input/input_init/pickup.000000001.data

By default, the model will write a new pickup file at the calendar end of each simulated year. The integer number associated with the pickup file (e.g., **000000001**) corresponds with the model time step at the moment of the snapshot. Each new pickup file will increment by approximately 8760 (there are approximately 8760 1-hour model time steps per year).

To restart the model from a pickup file other than **pickup.000000001.data**, you must (1) tell the model to use the time step corresponding with the integer of the pickup file and (2) disable the control adjustments to the model's initial conditions of **U,V,T,S**, and **ssh**. Both steps require modifying run-time namelist files in the **WORKINGDIR/ECC0V4/release4/namelist**/ directory.

To update the model's initial time step, change the parameter **nIter0** in the **data** namelist file. To disable the control adjustments to the model's initial conditions modify the **data.ctrl** namelist file. For users' convenience, we provide an example **data.ctrl** specifically for restarting from a different pickup file: **data.ctrl.restart**. When restarting the model, unlink the default **data.ctrl** and rename/copy **data.ctrl.restart** to **data.ctrl**.

7. Configuring custom diagnostic output

Various model fields (e.g., temperatures, salinities, velocities, fluxes) can be output by the model when re-running the simulation using the MITgcm's *diagnostic* package. The full list of pre-defined diagnostic fields that one can output is provided in here:

WORKINGDIR/ECCO-v4-Configurations/ECCOv4 Release 4/doc/available_diagnostics.log

Users can specify which diagnostic fields to output in the data.diagnostics runtime parameter file: WORKINGDIR/ECCOV4/release4/namelist/data.diagnostics

The diagnostic package can average fields over different time periods, provide snapshots of the model state, and even perform some statistical calculations. Interested users can even define their own diagnostics. More information about how to use the package can be found in *Chapter* 7 of the MITgcm user manual, "Diagnostics and I/O - Packages II, and Post-Processing Utilities": <u>https://mitgcm.readthedocs.io/en/latest/outp_pkgs/outp_pkgs.html</u>

8. Reproducing the "control run" aka "Iteration O"

To reproduce the first-guess un-optimized model solution, otherwise known as the control run or iteration 0, one must not apply control variable adjustments and only use first-guess atmosphere forcing, mixing parameters, and initial conditions. This can be done by modifying five name list files, which we provide in WORKINGDIR/ECCOV4/release4/namelist/ with the filenames ending with ".iter0". When producing the "control run", use these five modified name list files, but rename/copy them by removing ".iter0" in the filenames. In practice, it is a good idea to first save the original name list files to different files for possible optimized runs later. An example to do what is described above is shown in the following box.

```
cd WORKINGDIR/ECCOV4/release4/namelist/
cp data.ctrl data.ctrl.optimized
cp data.exf data.exf.optimized
cp data.gmredi data.gmredi.optimized
cp data data.optimized
cp data.optim data.optim.optimized
cp data.ctrl.iter0 data.ctrl
cp data.exf.iter0 data.exf
cp data.gmredi.iter0 data.gmredi
cp data.iter0 data
cp data.optim.iter0 data.optim
```

8.1 First-guess external forcing

The first-guess atmosphere forcing for V4r4 is from ERA-Interim, which one can find in **WORKINGDIR/ECCOV4/release4/input/input_forcing/unadjusted/.**

When reproducing the "control run", one needs to use the first-guess atmosphere forcing instead of the optimized forcing. To do this, one can modify the example PBS script (pbs_eccoV4r4.csh) at the end of this document by replacing

ln -s \${inputdir}/input_forcing/adjusted/eccov4r4* .

with

ln -s \${inputdir}/input_forcing/unadjusted/eccov4r4* .

8.2 First-guess mixing parameters

The first-guess mixing parameters are spatially uniform: diffKr = 1E-5 m² s⁻¹, kapgm = 1.D+3 m² s⁻¹, and kapredi = 1.D+3 m² s⁻¹.

8.3 First-guess initial conditions

The first-guess initial conditions are stored in the pickup* files, which are linked in the run script.

8.4 Running iteration 0

Except for modifications related to linking unadjusted forcing (Section 8.1), the same run script can be used to run iteration 0.

The control run has much larger mode-data difference, measured by the sum of weighted model-data squared, a.k.a., cost, than the optimized V4r4. Figure 1 shows the cost ratio of V4r4 relative to the control run. The total cost (the leftmost bar) of V4r4 is 45% of the control run cost.



Figure 1. Cost ratio: V4r4 divided by the control run. The leftmost bar is for the total cost and the other bars are for individual costs.

9. Concluding remarks

If you have any questions, please contact us at ecco-support@mit.edu.

You can also subscribe to the mailing list http://mailman.mit.edu/mailman/listinfo/ecco-support

10. Acknowledgements

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11. References

ECCO Consortium, Fukumori, I., Wang, O., Fenty, I., Forget, G., Heimbach, P., & Ponte, R. M. (2021, February 10). Synopsis of the ECCO Central Production Global Ocean and Sea-Ice State Estimate (Version 4 Release 4). <u>https://doi.org/10.5281/zenodo.4533349</u>

Wang, O. (2017). Instructions for reproducing ECCO Version 4 Release 3. Available at https://ecco.jpl.nasa.gov/drive/files/Version4/Release3/doc/v4r3_reproduction_howto.pdf.

Example PBS script (pbs_eccoV4r4.csh) for submission to the NASA Electra Supercomputer

```
#PBS -S /bin/csh
#PBS -l select=3:ncpus=40:model=sky_ele
#PBS -l walltime=24:00:00
#PBS −j oe
#PBS -o ./
#PBS -m bea
limit stacksize unlimited
module purge
module load comp-intel/2020.4.304
module load mpi-hpe/mpt.2.25
module load hdf4/4.2.12
module load hdf5/1.8.18_mpt
module load netcdf/4.4.1.1_mpt
module list
setenv LD_LIBRARY_PATH ${LD_LIBRARY_PATH}
setenv FORT_BUFFERED 1
setenv MPI_BUFS_PER_PROC 128
setenv MPI_DISPLAY_SETTINGS
set nprocs = 96
set basedir = ./
set inputdir = ../input/
if ( -d ${basedir}/run) then
echo 'Directory "run" exists.'
echo 'Please rename/remove it and re-submit the job.'
exit 1
endif
mkdir ${basedir}/run
cd ${basedir}/run
ln -s ../namelist/* .
ln -s ${inputdir}/input_init/error_weight/data_error/* .
ln -s ${inputdir}/input_init/* .
ln -s ${inputdir}/misc/tools/mkdir_subdir_diags.py .
ln -s ${inputdir}/data_constraints/data_error/*/* .
ln -s ${inputdir}/data_constraints/*/* .
ln -s ${inputdir}/input forcing/adjusted/eccov4r4* .
ln -s ${inputdir}/input_forcing/other/*.bin .
ln -s ${inputdir}/input_forcing/control_weights/* .
ln -s ${inputdir}/native_grid_files/tile*.mitgrid .
python mkdir_subdir_diags.py
cp -p ../build/mitgcmuv .
mpiexec -np ${nprocs} /u/scicon/tools/bin/mbind.x ./mitgcmuv
```