"Data sets used in ECCO Version 4 Release 3"

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Summary

The latest state estimate produced by the consortium for Estimating the Circulation and Climate of the Ocean (ECCO Version 4 Release 3 or V4R3 for short) is constrained by a variety of satellite and in situ ocean observations. Many of these data sets (e.g., satellite altimetry, sea surface temperature, in situ hydrography) are extensions of those used in earlier Version 4 releases described by *Forget et al.* (2015, 2016), but others (regional and global ocean mass from satellite gravity, satellite surface salinity, Arctic temperature and salinity profiles, sea-ice concentration, and global mean sea level) are newly introduced in V4R3. All data sets used in V4R3 are available with the solution output at ftp://ecco.jpl.nasa.gov/Version4/Release3/. A brief description of the data sets and the main processing applied to them is provided in this document, to complement full details of the V4R3 estimate discussed in *Fukumori et al.* (2017).

1 Basic Data Sets

All observations used as constraints in V4R3 are listed in Table 1. Several data sets used in ECCO Version 4 Release 1 (V4R1), restricted to the period 1992-2011, have been extended in time to cover the 1992-2015 period of V4R3, depending on availability at the time of computation. In addition, measurements that had not been employed previously have been introduced in the new estimate to better constrain the solution.

The new observations include GRACE-derived monthly ocean bottom pressure variations and global mean ocean mass estimates, altimeter-derived global mean sea level, Aquarius sea surface salinity, and additional (>100,000) in situ temperature and salinity profiles especially in the Arctic Ocean. Some of the observations used in V4R1 have also been replaced with alternate data sets in V4R3; updated observations include temperature and salinity climatology (World Ocean Atlas 2009) and mean dynamic topography (DTU13).

Description of the data sets used in V4R1 has already been provided in *Forget et al.* (2015). In the rest of this note, we provide relevant missing details on provenance and processing of all data sets used in V4R3 and listed in Table 1. Additional information on each data set is provided at ftp://ecco.jpl.nasa.gov/Version4/Release3/input_ecco/, where all data sets reside. In some cases, particularly for in situ data sets, full information on data provenance and processing is not available.

Included also in the description below are details on the weights used for most of the different data types. Individual constraints in the optimization have been scaled in V4R3 by their corresponding model area to account for the model's spatially inhomogeneous resolution. Specifically, prior uncertainties are normalized (divided) by the square root of the corresponding area of the model grid relative to its largest element (relative area). Such scaling assures that the objective function and its gradients, and thus the optimization, are not dependent on the particular choice of the model grid system.

Variable	Observations
Sea level	TOPEX/Poseidon (1993-2005), Jason-1 (2002-2008), Jason-2 (2008-2015), Geosat-Follow-On (2001-2007), CryoSat-2 (2011-2015), ERS-1/2 (1992-2001), ENVISAT (2002-2012), SARAL/AltiKa (2013-2015)
Global mean sea level	Average of mean sea level curves from AVISO, CSIRO, NOAA
Temperature profiles	Argo floats (1995-2015), XBTs (1992-2008), CTDs (1992-2011), Southern Elephant seals as Oceanographic Samplers (SEaOS; 2004-2010), Ice-Tethered Profilers (ITP, 2004-2011)
Temperature (moorings)	Beaufort Gyre, Davis Strait
Salinity profiles	Argo floats (1997-2015), CTDs (1992-2011), SEaOS (2004-2010)
Salinity (moorings)	Beaufort Gyre, Bering/Davis/Fram Straits
Sea surface temperature	AVHRR (1992-2013)
Sea surface salinity	Aquarius (2011-2013)
Sea-ice concentration	SSM/I DMSP-F11 (1992-2000) and -F13 (1995-2009) and SSMIS DMSP-F17 (2006-2015)
Ocean bottom pressure	GRACE (2002-2014), including global mean ocean mass
TS climatology	World Ocean Atlas 2009
Mean dynamic topography	DTU13 (1992-2012)

Table 1: Observations employed in V4R3. New items from V4R1 are indicated in red.

2. Data Sets Using Satellite Observations

2.1 Altimetry

(Data processed and generated by Charmaine King and Gael Forget)

The V4R3 solution uses RADS (Radar Altimeter Database System) satellite altimeter data described by *Scharroo et al.* (2013) and available at http://rads.tudelft.nl. The data base contains validated and cross-calibrated altimeter data products that are consistent in accuracy, format, correction and reference system parameters.

Along-track sea surface height anomaly fields from all satellites available were daily bin-averaged onto the V4R3 model grid using gcmfaces (*Forget et al.* 2015) and organized by year. Outliers were removed using a standard deviation scheme discussed by *Forget and Ponte* (2015). Missing values and land were masked with -9999. The names of the datasets with daily bin-averaged data used in V4R3 are:

RADS_TJ_mar2016_YYYY (where YYYY=1992:2015; includes Topex, Jason data);
RADS_GFO_C2_mar2016_YYYY (includes GFO, Cryosat-2 data);
RADS_ERS_ENV_SA_mar2016_YYYY (includes ERS, ENV, Saral data).

More details on the RADS data processing can be found at http://wwwcvs.mitgcm.org/viewvc/MITgcm/MITgcm_contrib/ecco_utils/input_ecco_processing/ (see file README_sla.txt for all the RADS corrections and flags applied to the data, and files under subdirectory code_sla/ for the scripts used in the data processing). An extensive discussion of weights used for the altimeter observations is given in *Forget and Ponte* (2015).

2.2 Global mean sea level

(Data processed and generated by C. Piecuch)

We use an ensemble-average global mean sea level curve, which is based on time series available from three different altimeter processing centers (AVISO, CSIRO, NOAA). Details of the original data and processing for each center are given in *Masters et al.* (2012). All the estimates used to produce this composite sea level curve are based on TOPEX/Poseidon and Jason-1 and Jason-2 missions and thus represent only average sea level within 66 degrees of the equator. The time series comprises 276 real monthly values (units of meters) over 1993-2015. A correction for glacial isostatic adjustment (GIA) due to changes in ocean basin shape, amounting to 0.3 mm/a, has been included. In addition, 60-day smoothing has been applied to cope with a spurious 59-day cycle in the data (*Masters et al*. 2012). The mean standard deviation of the three possible difference time series (AVISO minus CSIRO, AVISO minus NOAA, CSIRO minus NOAA) was 2.3 mm, based on the 60-day averages. The standard error was taken to be 3.25 mm, to account for the use of monthly data.

2.3 Ocean bottom pressure

(Data processed and generated by K. Quinn; see AER directory /home/kquinn/grace/ECCOwgts/output_ECCOgrids_JPL_RL05M.m)

GRACE data are from the JPL RL05 Mascon (Version 1) solution (*Watkins et al.* 2015) described in detail at http://grace.jpl.nasa.gov/data/get-data/jpl_global_mascons/, with center-of-mass and C20 (degree 2 order 0) coefficients replaced by more reliable non-GRACE estimates, and with GIA correction and the coastline resolution improvement (CRI) filter applied. The GRACE fields (GRACE_jpl_rl05m_withland_noNaN_yyyy) in the native mascon resolution (~300km) were interpolated onto the V4R3 model grid. Other pre-processing of the data included adding back the GAD model fields (*Flechtner et al*. 2015) and removing the spatial mean. Land and missing values were masked as –999.

Errors were estimated by comparing to iteration 0 values from 2003 through 2010 using method in *Quinn and Ponte* (2008). The GRACE error field (GRACE_jpl_rl05m_withland_err) is estimated from data and model fields that have been smoothed using the "diffusion" filter described in *Forget et al.* (2015; Appendix E), with an equivalent smoothing scale of 300km. (Note that, for consistency, file MITgcm/pkg/ecco/cost_gencost_bpv4.F, used to calculate GRACE cost term in V4R3 needs to have hard-coded smoothing of 300km also, instead of 500km used in previous releases.)

The global mean ocean mass (file GRACE_jpl_rl05m_SpatialMean.asc) was estimated by calculating the spatial mean of the same mascon fields described above. The mascon values do not include atmospheric mass contribution to ocean bottom pressure and are thus equivalent to mass variability resulting from net freshwater flux. Missing values are flagged as –999.

Error of 1.7 mm for the spatial mean was estimated as the standard deviation of the residual after removing trend, annual and semiannual components and accounting for the reduction in variance of a random distribution with the same fit (*Wahr et al.* 2006). This procedure will overestimate errors if geophysical signals are in the residual.

2.4 Mean dynamic topography

(Data processed and generated by K. Quinn; see AER directory /home/kquinn/MDT/ for files and other information)

Mean dynamic topography (MDT) field used was that produced at the Technical University of Denmark, DTU Space, named DTU13MDT. The field is based on the differencing of a mean geoid (EIGEN-6C3), from GRACE data (2003-11) and GOCE data (Nov 2009-May 2013), and a mean sea surface (DTU13MSS), from 20 years (1993-2012) of altimetry data, including Cryosat-2 data in the Arctic up to 88N and retracked Envisat, ERS-1 and ERS-2 data. Information on DTU13MSS used can be found at

http://www.aviso.altimetry.fr/fileadmin/documents/OSTST/2013/oral/Andersen_DTU13MSS.pdf

Information on previous MDTs produced by DTU and relevant for the DTU13MDT can be found at

http://www.space.dtu.dk/english/Research/Scientific_data_and_models/Global_Mean_Dynamic_topography

The original DTU13MDT data, provided on a 1-minute arc grid, was downloaded from ftp://ftp.space.dtu.dk/pub/DTU13/1_MIN/DTU13MDT_1min.mdt.nc, and binned onto the V4R3 model grid (mdt_dtu13.m) as done for previous MDT used in V4R1 (DOT2008a; *Forget et al.* 2015). The associated error field is a combination of the old error field used in V4R1, which was based on estimates of contributions from significant wave height, inverse barometer, and sampling errors, and a best guess based on comparisons between DTU13MDT, DOT2008a, *Maximenko and Niiler* (2005), and non-optimized ECCO MDTs (see discussion presented in the ECCO teleconference of October 24, 2014). The largest of the two error estimates is chosen locally and the results are smoothed over 300km. Error poleward of 88N latitude is set to 50 cm to reflect the complete lack of altimeter data.

2.4 Surface salinity (Aquarius)

(Data processed and generated by Nadya Vinogradova)

Aquarius surface salinity data are Level 3 monthly gridded fields (Version 3), originally obtained from https://podaac.jpl.nasa.gov/SeaSurfaceSalinity/Aquarius. (Data has since been retired and resides at ftp://podaac-ftp.jpl.nasa.gov/allData/aquarius/retired/L3/mapped/V3/monthly/SCI/ now). The fields are provided on a 1° horizontal grid as a combination of measurements from ascending and descending tracks from the three radiometer beams. The fields are unsmoothed, i.e., typical 2° smoothing scale is not applied.

Data used in V4R3 span the period September 2011 through December 2013. (At the time of writing, Aquarius data is available up until May 2015, when the mission came to an end.) The Aquarius fields are derived using Aquarius version 3.0 algorithm. For details, see documentation (AquariusUserGuide_DatasetV3.0.pdf) available at ftp://podaac-ftp.jpl.nasa.gov/allData/aquarius/docs/v3/.

The Aquarius errors are estimated by comparing satellite salinity observations with in situ data and output from the V4R3 iteration 0 using methodology described in *Vinogradova et al.* (2014). For V4R3, aside from errors for salinity anomalies from the time mean, separate bias errors were also estimated based on differences in time means of in situ and satellite data sets. Both time-mean and time-variable errors were then floored at a minimum of 0.1 psu, after considering overall Aquarius uncertainties provided by the mission and initial cost statistics. Derived Aquarius data errors are less than the total allocation errors for the Aquarius mission accuracy requirements in low and mid-latitudes. For more information on consistency of Aquarius salinity with in situ observations see also *Lee* (2016).

2.5 Sea surface temperature (SST)

(Data processed and generated by Charmaine King and Gael Forget)

Monthly SST data from the NOAA Optimum Interpolation Sea Surface Temperature Version 2 (NOAA_OI_SST_V2) product were obtained from the NOAA/OAR/ESRL PSD, Boulder, Colorado, USA (http://www.esrl.noaa.gov/psd/data/gridded/data.noaa.oisst.v2.html). The product consists of an optimally interpolated mixture of satellite and in situ observations following the methodology of *Reynolds et al.* (2002).

The monthly SST data, originally on a 1° horizontal grid, are mapped onto the V4R3 model grid using gcmfaces (*Forget et al.* 2015) and organized by year. Missing values are masked with –9999. Data files used in V4R3 are named reynolds_oiv2_r1_YYYY, and scripts used to pre-process and create these files are available at http://wwwcvs.mitgcm.org/viewvc/MITgcm/MITgcm_contrib/ecco_utils/input_ecco_processing/. Errors for these SST fields were set to a globally constant value of 0.5 degC.

2.6 Sea-ice concentration

(Data processed and generated by Ian Fenty)

Daily sea-ice concentration estimates used are based on the “Merged GSFC NASA Team/Bootstrap daily sea ice concentrations” product included as part of the “NOAA/NSIDC Climate Data Record of Passive Microwave Sea Ice Concentration, Version 2” National Snow & Ice Data Center (NSIDC), Boulder, Colorado Dataset G02202 available at http://nsidc.org/data/G02202#cdr_alg (*Meier et al*. 2017, *Peng et al*. 2013). As per the data description, “*the GSFC-merged concentrations are produced from the final, fully quality-controlled NASA Team and Bootstrap concentrations produced at GSFC. These fields include thorough quality control, including manual correction/replacement of bad values (for example, false ice due to weather effects over the ocean), and spatial or temporal interpolation to fill in missing values. It encompasses the entire SMMR-SSM/I-SSMIS record from late 1978 to present”*. See the NSIDC dataset web site for details on microwave sensor satellites and retrieval algorithms used for this product.

Files NOAA_NSIDC_DAILY_MAPPED_TO_LLC90_YYYY contain the daily data mapped to the V4R3 grid and organized by year, as indicated by the YYYY suffix (1992-2015). The following directory has the scripts used to process the daily and monthly versions of these observations:
https://github.com/ECCO-GROUP/OBS_DATA_PROCESSING/tree/master/sea_ice/concentration/ECCOv4R3_NOAA_NSIDC_ClimateDataRecord_V2_Merged_GSFC_product

Sea ice concentration data was not used to constrain V4R3 directly, as its contributions to the cost function were set to zero. Instead, model-data misfits were used to estimate penalties in heat content that were applied to the surface layer to create or melt ice, which improve ice concentration estimates (*Fukumori et al*., 2017).

3. In Situ Data Sets

A general presentation of in situ observations used in V4R1 and of the underlying MITprof format is available in *Forget et al.* (2015). The current version of the MITprof toolbox is available at https://github.com/gaelforget/MITprof. The various in situ datasets have been updated and extended for use in V4R3 as described below.

To limit computational burden for users, the MITprof toolbox discretizes profile measurements, such as Argo profiles, to 95 standard depth levels by default. However, the vertical resolution afforded by such discretization is higher than that of the current model resolution, resulting in correlated model-data differences. To minimize such correlation, profile measurements in V4R3 were decimated among these levels to no more than the model’s vertical grid resolution.

Data errors for the time-dependent hydrographic profile costs were also revised from those employed in V4R1. Errors associated with meso-scale variability not resolvable by the Version 4 model were estimated using the 3-day average output from a nominal 1.2 km horizontal resolution, unconstrained forward MITgcm simulation on the LLC4320 grid (courtesy Dimitris Menemenlis). The spatial patterns and magnitudes of these LLC4320 variations were found to agree favorably with data errors used in V4R1 (derived by G. Forget using in situ profile data, following *Forget and Wunsch*, 2007) with the exception of Arctic and Southern Oceans, where in situ profile data are relatively sparse. In the Arctic and Southern Oceans, errors used in V4R1 were replaced with the LLC4320 variance in V4R3. In mid and low latitudes, the V4R3 hydrographic error field is set to be the maximum of the LLC4320-derived and in situ-derived fields.

Data errors for the time-invariant hydrographic profile costs were estimated from those for the time-dependent profile costs by assuming that there is a maximum of nine independent samples for each geodesic bin (*Fukumori et al*., 2017).

3.1 Climatology (temperature and salinity)

(Data processed and generated by Gael Forget and Ou Wang)

Temperature and salinity climatological fields are based on the World Ocean Atlas 2009 (WOA09; *Locarnini et al.* 2010, *Antonov et al.* 2010). Monthly data were downloaded from the NOAA National Oceanographic Data Center (NODC) site https://www.nodc.noaa.gov/OC5/WOA09/pr_woa09.html and mapped onto the V4R3 grid. Files T_monthly_woa09 and S_monthly_woa09, S_monthly_woa09 and S_monthly_woa09 with temperature and salinity fields, respectively, were obtained from MIT (/net/nares/raid11/ecco-shared/ecco-version-4/input/input_hydrogr_etc/), and values for the upper 10 model levels (surface to ~100 m) at latitudes poleward of 65N and 55S were masked out. Weights used for the climatology were the same as used for other in situ temperature and salinity data.

3.2 CTD and XBT (temperature and salinity)

(Data processed and generated by Gael Forget and Ou Wang)

Individual temperature and salinity CTD profiles and temperature XBT profiles available from the World Ocean Database at NODC were also used, in addition to the WOA09 climatology. Periods covered by the CTDs and XBTs are given in Table 1. Apart from decimation of vertical levels to the model grid resolution, these data are the same as used in V4R1 (*Forget et al.* 2015).

3.3 Argo floats (temperature and salinity)

(Data processed and generated by Gael Forget and Ou Wang)

Data from Argo floats were originally downloaded from the data center supported at IFREMER (http://www.argodatamgt.org/) for use in V4R1. Later on (February 2016) an update was done at MIT to include profiles through the end of 2015. At that time, the MITprof toolbox was also updated and all profiles were re-processed to (1) benefit from the latest delayed mode quality control performed by the Argo team, (2) update the treatment of Argo quality controls, and (3) use bilinear interpolation rather than nearest neighbor interpolation to create the weight profiles. The reprocessed Argo data sets were released as part of ECCO Version 4 Release 2 and later modified by Ou Wang for use in V4R3 as explained at the beginning of this section.

3.5 CLIMODE (temperature and salinity)

(Data processed and generated by Charmaine King and Gael Forget)

These data include temperature and salinity CTD profiles and temperature profiles from bobber floats, both collected in 2006 and 2007 during the CLIMODE field program in the subtropical North Atlantic (*Marshall et al*., 2009). Data was originally obtained directly from CLIMODE scientists Lynn Talley and David Fratantoni, but full provenance information is not available. In addition, it is possible that some or most of the CTD profiles from CLIMODE are repeated as part of the World Ocean Database CTD data described in section 3.2.

3.6 ICES (temperature and salinity)

(Data processed and generated by Ian Fenty)

Temperature and salinity profiles were obtained from the International Council for the Exploration of the Sea (ICES; http://ices.dk/Pages/default.aspx) database available at http://ices.dk/marine-data/data-portals/Pages/ocean.aspx. The ICES data set focuses on high latitudes but duplication in other data sets in section 3.2 cannot be excluded.

3.7 Ice-Tethered Profilers (temperature and salinity)

(Data processed and generated by An Nguyen and Gael Forget)

Temperature and salinity from ice-tethered profiler (ITP) measurements collected over the period 2004-2011 were obtained directly from J. Toole and M.-L. Timmerman (*Toole et al.* 2011). Data used is the same as in V4R1 apart from the differences in processing already discussed in the context of the Argo float data (section 3.3) and additional updates to the hydrographic uncertainty fields by An Nguyen and Ian Fenty using the global LLC4320 temperature and salinity variance.

3.8 SEaOS (temperature and salinity)

(Data processed and generated by Fabien Roquet, others at MIT over several years)

Vertical profiles collected by elephant seals in the Southern Ocean were originally compiled by Fabien Roquet with the help of others over an extended period of time at MIT (*Roquet et al.* 2011) and details of the processing are not well documented. Data used is the same as in V4R1 apart from differences in processing already discussed in the context of Argo floats (section 3.3).

3.9 Arctic moorings (temperature and salinity)

(Data processed and generated by An Nguyen)

Beaufort Gyre mooring data (at hourly frequency) were downloaded from http://www.whoi.edu/beaufortgyre and averaged to daily and interpolated to the generic 85-depth levels in the profile package. “Uncertainties” were calculated using the hydrographic variance (after seasonal cycle removed) at each of the four mooring sites.

Fram Strait mooring data from 17 mooring sites at hourly frequency were obtained from Wilken von Appen (at the time a postdoc at AWI working with Ursula Schauer and Agnieska Beszczynska-Möller). References for the data should be *Beszczynska-Möller et al.* (2012). Data were averaged to daily and re-located to nearest depth levels. "Uncertainties" for hydrography were derived as described above. (Uncertainties for eastward and northward velocities were also calculated using variance but not yet rigorously tested. To properly use the velocity as constraint, it is likely necessary to split the cost into mean and anomalies.)

Davis Strait mooring data at daily frequency were obtained from Beth Curry (*Curry et al*. 2014). Processing of the hydrographic data was done the same way as described above. Velocity data were not used.

Bering Strait mooring data were obtained from Rebecca Woodgate (*Woodgate et al*. 2011) and processed the same way as described above.

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