

WP2500 Deliverable:

Toolbox Verification and Validation Report

Version: 2; 19 August 2011

Ref:

ESA/XGCE-DTEX-EOPS-SW-09-0001 "GUTS Phase 3: GUT Development and Supporting Scientific Studies"

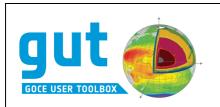
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WP2500: "Evaluation and Testing"

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DOC	UMENT	CHANGE	ELOG	_	
Rev.	Date	Sections modified		Comments	Changed by
0	Mar 2011				
1	June 2011	All			HMS
2	Aug 2011	Title Page 3.1.1 3.2 3.3.1 3.3.2 3.3.3 3.3.4 5.11.2	Addition of Version No Fig 1 & Fig 2, coastline changed to white DO and SHP defined Correct statistics included in Results MDTC defined Statistics of speed and direction calculations provided ACC changed to Antarctic Circumpolar Current typo correction to punctuation typo correction in fig 5 caption (added 'one') typo correction in fig 6 caption (and → an) New section added to validate spline interpolation Renumbered from 3.3.2 Added reference for GMT Added statistics on track data Renumbered from 3.3.3 typo corrected (Bougier → Bouguer)	Modified in response to ESA review	HMS



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Applicable and Reference Documents

AD1 XGCE-DTEX-EOPS-SW-09-0001: "GUTS Phase 3: GUT Development and Supporting Scientific Studies". Response to ESA Intended Extension to ESRIN/Contract No. 19568/06/I-OL Statement of Work XGCE-DTEX-EOPS-SW-09-0001, 26 November 2009.

ESA-GUT2-SAD-001. GUT2 Technical Specification and Architectural Design v1.1, 21 September 2010.

AD3 ESA/XGCE-DTEX-EOPS-SW-04-0001 "GOCE User Toolbox Specifications (GUTS)", GUTS Final Report, 20 July 2007.

ESA/XGCE-DTEX-EOPS-SW-04-0001 "GUTS Phase 2: GUT Implementation and Supporting Scientific Studies", GUTS Final Report, 21 August 2009.

GUT Tutorial, v5, 2011-03-22

"GOCE High level processing facility - GOCE Level 2 Data Handbook", GO-MA- HPF-GS-0110, iss. 4.1, 23-June-2010

RD2 ESA-GUT2-TP-001. GUT2 Software Test Plan v1.4, 24 March 2011.

RD3 "GUT User Guide and Algorithm Descriptions", ESA-GUT-AD-001, v2.0, 2011-03-09

"GUT Installation Guide", v2.0, 2011-03-17 RD4

Abbreviations

ADT	Absolute Dynamic Topography
CLS	Collecte Localisation Satellites
DO	Degree and Order
GOCE	Gravity and Ocean steady-state Circulation Explorer
GUT	GOCE User Toolbox
HPF	High level Processing Facility
MDT	Mean Dynamic Topography
MSS	Mean Sea Surface
NOCS	National Oceanography Centre, Southampton
S&T	Science and Technology, Delft
SPH	Spherical Harmonic Potential
SLA	Sea Level Anomaly



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1 Introduction

This document presents the results of the GUT v2 testing and validation carried out under WP2500. The testing and validation was carried out in order to evaluate the ability of the toolbox to:

- Reproduce the validated results generated by the v1 release of the software using v2 of the software.
- Validate the results generated by the new options available in the v2 release, as specified in [AD2], in particular:
 - o Validate the new functionality to add or subtract a constant from a grid function
 - apply a height correction term to geoid height field
 - o generate a Grid Function from a windowed bicubic spline interpolation of a Grid Function at positions specified by a Grid
 - generate an Anisotropic Filter Kernel defined by a meridional scale length and an orthogonal scale length (i.e. east-west in the equator)
 - generate a Filtered Track Function by convolution with a Spatial Filter Kernel
 - store/read geostrophic velocities as a magnitude/direction pair.
 - perform statistics on limited regions of a Grid Function specified by longitude/latitude ranges

The correctness and completeness of the toolbox documentation was also assessed.

2 Software Test Plan

The software was released with a software test plan [RD2], included as Annexe A in this report.

This test plan was specified by S&T and conformance with the test plan ensures that the toolbox release conforms with those aspects of the technical specification and architectural design document [AD2] that were specified as requiring a specific test to be implemented.

The current release of the software has passed all tests on the following platforms:

- MacOS X (10.6) using source distribution
- Linux (Ubuntu) using source and binary distributions
- Linux (SUSE Enterprise Desktop 10) using source distribution
- Windows XP using Windows32 binary distribution
- Linux debian (4.0) using src distribution (development system)

The final testing of v2.0 of the software revealed an error in the implementation of the application of the geoid height correction file. By default, the GUT v2 supplied workflow incorrectly scales the input height correction file by a factor of 1/100. This error was introduced by the inability of v1 to correctly recognise the units of the input file (cm). Instead, the units were provided as 'm', and a scaling factor of .001 applied to convert from cm to m. As GUT v2 correctly assigns the units, the scaling factor creates an error. This has been correctly in the beta v2.1 version of GUT.

No remaining issues were identified by the formal testing.

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3 Validation Testing Protocols

The GUT is required to provide a scientific research tool that can be used to generate geophysical products. The approach taken for validation of v2 of the toolbox was the same as that used for v1: to use the toolbox to generate results that were comparable to those generated using existing software, currently in use in the research community, from datasets similar to those to be used within the toolbox. In the first instance, the toolbox is expected to reproduce the specific gridded products released by the HPF, in particular the geoid height, gravity anomaly and vertical deflections of gravity provided in the GOCE level two products. Additional test datasets and workflows used in the validation were designed to allow the recreation of results equivalent to those presented in the GUT tutorial [AD5]. All data provided for testing as ASCII or binary format were first translated to NetCDF format using MATLAB and then to GUT compliant NetCDF format using the appropriate GUT import workflow, for use in the validation process. The resultant files were read into MATLAB to confirm that the GUT import function had retained the original data values.

Where single workflows are provided with the GUT distribution to carry out a specific activity, these have been used in generation of the validation report. In other cases, workflows have been used in sequence to generate an equivalent product.

The following sections present the results of the validation exercise for a number of required activities. The results obtained, and comparisons to results generated using existing software, will be presented.



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3.1 **Geoid and Gravity Field Computations**

3.1.1 Calculation of a gridded geoid height field from spherical harmonic potential coefficients

An initial test was performed to reproduce the example gridded field generated by the HPF and provided in the apriori GUT_GOCE2_Example file, using the spherical harmonic potential coefficients provided in the same input file, as was done for the v1 validation. The results were identical to those performed using v1.

Validation against HPF gridded geoid field

A validation of the v2 GUT was also carried out using the second release of the GOCE data the direct method files were chosen for this validation. The workflow requires the use of GUT to extract the pre-computed (HPF) grid, and compare this to the geoid heights calculated on the same grid using GUT.

Input file: GO_CONS_EGM_GOC_2_20091101T000000_20100630T235959_0002.DBL

Workflow:

```
gut import_gf
      -InFile GO_CONS_EGM_GOC_2__20091101T0000000_20100630T235959_0002.DBL
      -PQ geoid_height -OutFile GUT_GOCE_Direct_geoid_grid.nc
gut geoidheight_gf
      -InFile GO_CONS_EGM_GOC_2__20091101T0000000_20100630T235959_0002.DBL
      -Gf GUT_GOCE_Direct_geoid_grid.nc
      -OutFile GUT_GOCE_Direct_geoid_calc.nc
```

Output Files: GUT_GOCE_Direct_geoid_grid.nc and GUT_GOCE_Directe_geoid_calc.nc

Results

The mean difference between the fields is less than 10⁻⁵ m, with a range of ±6×10⁻⁴ m, ie better than 1 mm, with a random distribution of the differences (Figure 1). As mentioned in the validation report for v1 of the toolbox, the HPF gridded field is only reported to 1 mm, limiting the accuracy of the comparison possible. As the toolbox and the HPF use the same method of geoid height calculation, there are no reference ellipsoid or tide system transformations required in this calculation and the full degree and order of the input files are used in the expansion, the result validates the basic geoid height calculation.

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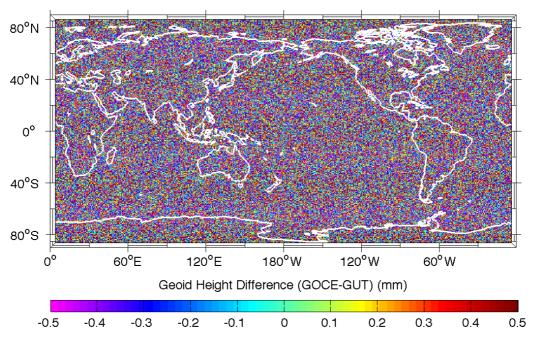


Figure 1: Difference between geoid height calculated using the toolbox from release 2 of the GOCE Direct Method SHP and the release 2 of the GOCE Direct Method gridded field, imported using the toolbox

Validation with geoid height correction file

GUT v1 was not able to incorporate geoid height correction files as a default action. Instead, as outlined in the validation section of the GUT final report [AD4], a sequence of workflows could be used to apply a geoid height correction. A single workflow has been included in GUT v2 to facilitate this process. As mentioned in §2, the v2 release of the software has an error in the workflow: a scaling factor of 0.01 was erroneously introduced into the height correction field. In order to test the workflow, as input, we used a version of the EGM96 correction coefficients file provided in cm, but (incorrectly) described as having units of m. We then created a correctly scaled version of the coefficients and repeated the multi-step approach used in [AD4].

We used the EGM96 spherical harmonic coefficients, the height correction spherical harmonic coefficients and the 15-minute gridded geoid height field, calculated on WGS84, available from:

http://earth-info.nga.mil/GandG/wgs84/gravitymod/egm96/egm96.html. The processing steps were:

- Convert the egm96 potential coefficients ascii file (egm96), geoid correction coefficients ascii file (corrcoef) and binary 15 minute gridded, height corrected geoid (WW15MGH.DAC) into netCDF format using matlab scripts.
- Import these NetCDF files into GUT format using import_shp (egm96 -> egm96_coef_wgs84_tide_free.nc), import_shf (corrcoef -> egm96_coef_corr_cm.nc), scale_gf (egm96_coef_corr_cm.nc -> egm96_coef_corr.nc) and import_gf (WW15MGH -> egm96_wgs84_tide_free.nc)



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- Compute the corrected geoid from the SHP to DO 360 and the height correction file (in cm) on the egm96 15 minute grid using the geoid with height correction workflow.
- Compute the raw geoid from the SHP on the same grid.
- Compute the height correction on the same grid (using the correctly scaled coefficients)
- Add the correction field to the geoid height

Input files: egm96_coef_wgs84_tide_free.nc, egm96_coef_corr_cm.nc, egm96_coef_corr.nc

Original Output File: egm96_wgs84_tide_free.nc

Workflow:

```
gut geoidheightcorrection_gf -InFile egm96_coef_wgs84_tide_free.nc
    -InFileCorr egm96_coef_corr_cm.nc -Gf egm96_wgs84_tide_free.nc
    -OutFile egm96_wgs84_TideFree_with_corr.nc

gut geoidheight_gf -InFile egm96_coef_wgs84_tide_free.nc
    -Gf egm96_wgs84_tide_free.nc
    -OutFile egm96_wgs84_TideFree_calc.nc

gut shf2gf -InFile egm96_coef_corr.nc
    -Gf egm96_wgs84_tide_free.nc -OutFile egm96_wgs84_height_corr.nc

gut add_gf -InFileLhs egm96_wgs84_TideFree_calc.nc
    -InFileRhs egm96_wgs84_height_corr.nc
    -OutFile egm96_wgs84_TideFree+corr.nc
```

New Output File: egm96_wgs84_TideFree_with_corr.nc, egm96_wgs84_TideFree+corr.nc

Results

The rms difference between the two fields generated by GUT (egm96_wgs84_TideFree_with_corr.nc and egm96_wgs84_TideFree+corr.nc) is 7.83×10^{-16} m, with a mean of 7.83×10^{-20} m.

There is a mean difference between the original NGA/NASA pre-calculated geoid height field and the GUT calculated fields of 53 cm, which corresponds to the bias applied to the NGA/NASA pre-calculated geoid height field to account for the difference between the WGS84 ellipsoid and the 'true' best fit reference ellipsoid (see http://earth-info.nga.mil/GandG/wgs84/gravitymod/egm96/egm96.html for more details). This bias can be removed from the EGM96 file using the new GUT workflow, addscalar_gf to give the difference plot (Figure 2). After adding the scalar, the mean difference of the NGA/NASA pre-calculated geoid height field is reduced to 0.015 mm and the rms difference is 2.9 mm. The range of the GUT calculated field is offset by 0.53 and, as expected, the other fields (variance, rms) of this field remain unchanged.

Workflow:

```
gut addscalar_gf -InFile egm96_wgs84_tide_free.nc -InScalar 0.53
    -OutFile egm96_wgs84_tide_free_offset.nc
```

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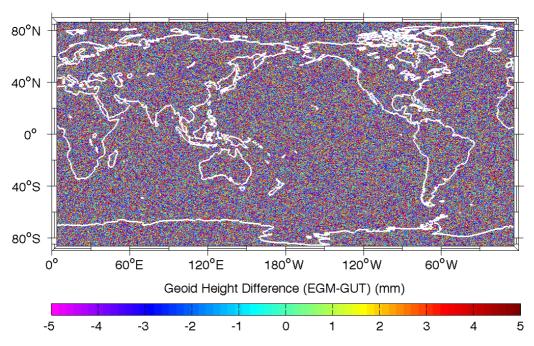
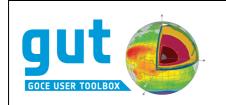


Figure 2: Difference between EGM96 geoid height provided by NGA/NASA, and that calculated by GUT from EGM96 gravity model coefficients, including geoid height correction coefficients (53cm bias removed).

Note on calculation time: The generation of the EGM 96 15-minute grids (using geoidheight_gf and shf2gf) to DO 360, each took approximately 4 minutes when run on a 64 bit linux machine, with 2 6-core 2.8GHz processors. This was an acceptable wait time, but probably at the limit of user acceptability.

An attempt was made to use the EGM08 model, to DO 2190, to calculate a 2.5 minute global grid, for comparison with the pre-computed EGM08 grid (see http://earth-info.nga.mil/GandG/wgs84/gravitymod/egm2008/egm08_wgs84.html). After 2 days, on the same machine, the calculation had only reached 65/4321 complete. If the toolbox is to cope with the demands of higher DO models, and the need for higher resolution outputs, these computation times will need to be addressed.



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3.2 Dynamic topography derived quantities

The absolute geostrophic circulation is computed in the Gulf Stream area on June 7th 2006 from a grid of absolute dynamic topographies (ADT). The ADT map was computed by adding a SLA map to an MDT.

The new workflow to allow direct computation of velocity as a speed and direction pair, rather than as separate North and South components was tested against the original workflows. In addition, the import2_gf was used to generate a single file containing both the North and East components of the velocity, and this file was used in matlab to generate speed and direction pairs.

Input files: adt_mdtc_A_max.nc

Original Output File: avel_mdtc_A_max.nc

Workflow:

```
gut gsveast_gf -InFile adt_mdtc_A_max.nc
        -OutFile AbsGeosVel_east.nc
gut gsvnorth_gf -InFile adt_mdtc_A_max.nc
        -OutFile AbsGeosVel_north.nc
gut import2_gf -InFile1 AbsGeosVel_east.nc
        -InFile2 AbsGeosVel_north.nc -OutFile AbsGeosVel_ne.nc
gut gsvdirectionspeed_gf -InFile adt_mdtc_A_max.nc
        -OutFile AbsGeosVel_ds.nc
```

New Output Files: AbsGeosVel_ne.nc, AbsGeosVel_ds.nc

Results

The speed and direction values calculated within matlab from the North and East velocity components (ie speed calculated using $\sqrt{\text{(eastward_velocity}^2 + northward_velocity}^2)}$ and direction calculated using arctan(northward_velocity/eastward_velocity) gave identical results to the values determined with GUT using the gsvdirectionspeed_gf workflow for speed (mean=0, rms=0) and for direction were within the machine calculation precision (mean=1.2777×10^{-16°} rms = 9.185×10^{-15°}).

Note on usability of output files: It was noted during the process, that the subtract_gf and stats_gf workflows could only be used to generate differences of, and to supply the statistics of, the first variable in the GUT dataset. Hence, it was simple to compare the speeds from two calculations, but to compare the directions (eg determined using two different input datasets), it is necessary to generate the two GUT files containing speed and direction, then use the import_gf on each of these, with the -PQ option set, to generate single variable files containing the directions. The subtract_gf can then be used on these files, but the speed and direction data have been split.

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3.3 Additional Functions

3.3.1 Anisotropic Filter

Release 2 of the toolbox introduced the option of using an anisotropic filter for both grid and track functions. All tests were carried out using the Gaussian filter, as other filters use the same function for determining search radius.

An initial test was made to ensure that using an anisotropic filter with both latitude and longitude filter radius set equal would result in identical output files. Both 222 km and 444 km filter radius values were set and generated identical output files.

Data generated by an independent fortran program were then used as a reference for further comparisons. The investigated filters were: 222km isotropic Gaussian filters, as a baseline for the two different processing methods, then 222x444km and 444x222km anisotropic filters. A land mask was generated from the original output files, and this was applied to the input MDT file to prevent contamination of the ocean values. **Note** – the notation in the filenames is radius_lonxradius_lat.

Input files: pw_mdt_GDIR2_L240.nc

Original Output File: pw_mdt_GDIR2_L240_agf_222x222km.nc pw_mdt_GDIR2_L240_agf_222x444km.nc pw_mdt_GDIR2_L240_agf_444x222km.nc

Workflow:

New Output Files: filt_spatial_222.nc filt_spatial_444x222.nc filt_spatial_222x444.nc

Results

The 222km isotropic filters (Figure 3) produced virtually identical results over the ocean. A very small number of points (approximately 20) near the northern limit of the grid had differences of up to +/-1 mm, where defining a latitudinal filter length becomes questionable. Everywhere else the results were within +/-0.1 mm – the reported accuracy of the original data files.



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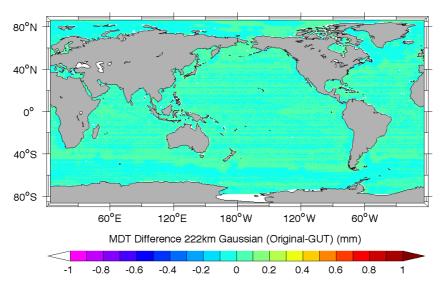


Figure 3: Difference between MDT fields filtered using a 222km isotropic Gaussian filter using original program and the same field filtered using GUT.

When results were compared for the anisotropic filtering, the results showed significant differences. The fields produced for a 222x444 km filter using the toolbox appear very similar to those using the fortran routines (Figure 4 top and middle). However, the difference between the two fields (Figure 4 bottom) ranges between -9.1 & 18.2 cm, with a rms difference of 1.7 cm. The largest differences are, again, towards the poles, where definition of ranges in latitude / longitude terms becomes somewhat arbitrary. However, it can be clearly seen that the differences are also concentrated on the areas of strongest signal - especially the Antarctic Circumpolar Current, but the Gulf Stream, Kuroshio and Agulhas can also be clearly seen. Even in quiet, low latitude areas of the ocean (see Figure 5, top) there is clear structure in the difference, although here the difference is a few mm, rather than cm. A very similar pattern can be seen for a 444km x 222km filter (see Figure 5, bottom), although here the differences are slightly lower(-2.7 cm - 6.1 cm, 0.5 cm rms). It appears as if the toolbox is applying a higher level of smoothing than is being applied by the fortran routines. The relative differences between the fortran and GUT version for the two different filters selected, is due to the general zonal nature of the global ocean currents, which accentuated the relative over-filtering in GUT more when the zonal length scale used is shorter.

It is not clear whether the problem is that GUT is applying too much smoothing, or that the fortran routines are not applying sufficient smoothing. There is an incompatibility in the fortran routines, in that using an isotropic filter does not produce an identical field to using an anisotropic filter with equal latitude and longitude ranges selected. The difference between the anisotropic case and the isotropic case (Figure 6) gives a very similar result to the difference between the GUT and the fortran routines both using anisotropic filtering. The difference range from -3 cm to 9.4 cm, with an rms of 0.7 cm, so are lower, but have similar structure.

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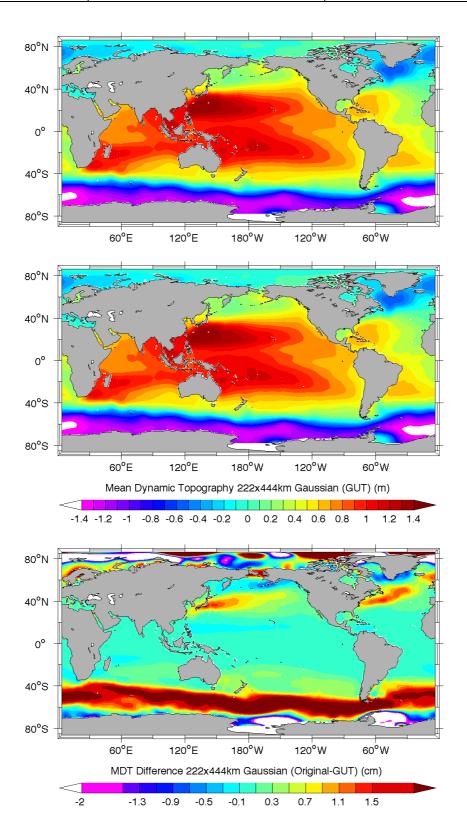


Figure 4 MDT filtered using 222km x 444km (zonal x meridional) anisotropic filter, using the fortran routines (top) and using GUT (middle) and the difference (bottom)



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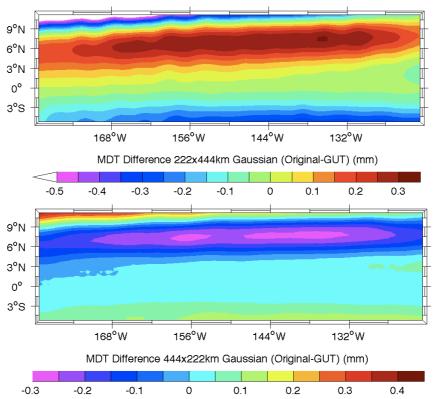


Figure 5 Difference between a Central Pacific MDT filtered using the fortran routines and one filtered using GUT with a 222km x 444km (zonal x meridional) (top) and a 444km x 222km anisotropic filter (bottom)

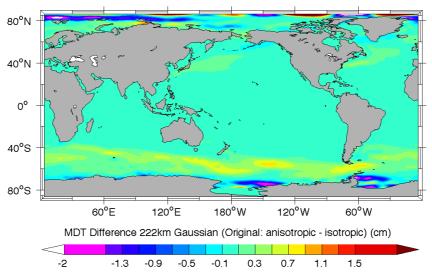


Figure 6 Difference between an MDT filtered using a 222km x 222km anisotropic filter and one filtered using a 222km isotropic filter, using the fortran routines

So far, it has not been possible to identify the source of this difference (between the isotropic and anisotropic filtering). Given the differences are still small, and that there is some uncertainty as which of the filtering methods is 'more correct', it appears that the toolbox anisotropic filtering in the toolbox is operating as defined in the handbook.

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3.3.2 Carry out spline interpolation

To validate the spline interpolation introduced in v2 of GUT, the adapt_gf workflow was used to generate a mean dynamic topography grid using both the linear and spline interpolation options, from a $\frac{1}{4}$ ° original grid to a 0.125° grid. The resultant fields were compared to fields generated within matlab using the matlab griddata routine, and the linear and cubic methods.

Input files: adt_mdtc_A_max.nc

Workflow:

```
gut adapt_gf -InFile input/adt_mdtc_A_max.nc -R 290/310/35/45 -I
    0.125/0.125 -Ellipse TOPEX -OutFile adt_linear.nc
gut adapt_gf -InFile input/adt_mdtc_A_max.nc -R 290/310/35/45 -I
    0.125/0.125 -Ellipse TOPEX -IntAlg spline -OutFile adt_spline.nc
```

New Output Files: adt_linear.nc, adt_spline.nc

Results

The GUT and matlab interpolations (for both linear and spline interpolation) produce very similar looking resultant fields (eg. See the spline interpolations in Figure 7), with very similar height distributions. The difference between the two fields only exists at grid-scale resolution, and is due to minor differences in the calculation methods used. The difference only ranges between -20.6 and 23.3 mm for the spline interpolations, which is a small difference given that the area selected has very strong surface height gradients (almost $0.5 \, \text{m}$ / degree in some areas), which will highlight even minor differences in the interpolation. The mean difference between these two fields is -0.01 mm, with an rms difference of only 1.8 mm.

The spline fit produces a different result to the linear fit, the two GUT calculated fields having a mean difference of 0.06 mm (ie the interpolation does not introduce a significant bias) but an rms difference of 6.1 mm. This is very similar to the difference between the matlab linear and spline interpolated fields (mean difference 0.05 mm, rms difference 5.2 mm)



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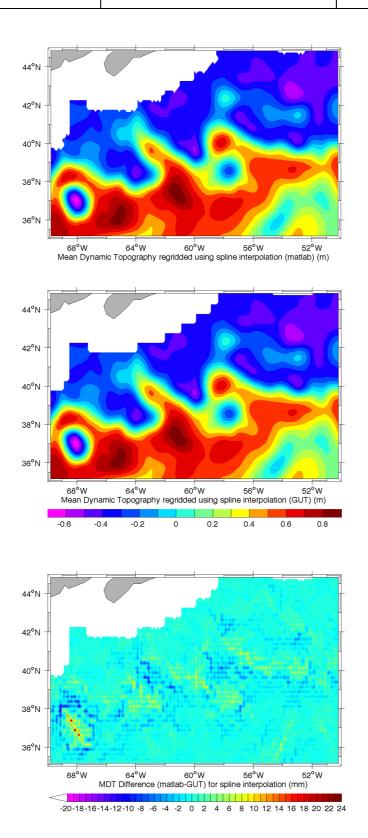


Figure 7 A regional MDT generated by spline interpolation in matlab (above), using GUT (middle) and the difference (bottom)

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3.3.3 Apply a filter to a track function

To test the track filtering options, a track of Envisat altimetry data (see Figure 8 for the track location) was converted to NetCDF and used as input. Two versions of the data were used, a complete track, with only short data gaps (envisat_sgdr_gut.nc) and a version containing only coastal data (envisat_cgdr_gut.nc), which therefore had long data gaps. The GMT filter1d routine (http://gmt.soest.hawaii.edu/) was used, with a Gaussian filter, Full Width Half Maximum scale of 400 km. GMT does not filter directly to the original data points, but re-samples onto a regular spaced track. The sampling selected was 7.3899 km along track distance – which produces a track very close to the original locations. The full dataset was also filtered using a simple boxcar (200 km Half Width) filter.

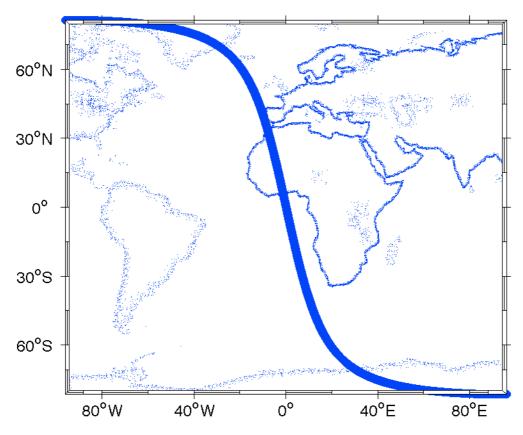
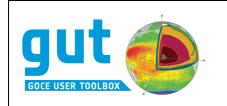


Figure 8 Location of ENVISAT altimeter track used for filtering



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Input files: envisat_sgdr_gut.nc, envisat_cgdr_gut.nc

Original Output Files: envisat_sgdr_gmt_filt1d.out, envisat_cgdr_gmt_filt1d.out

Workflow:

```
gut import_tf -InFile envisat_sqdr_gut.nc -Ellipse WGS84rev1
    -T mean-tide nc -OutFile envisat_sqdr_qut_tf.nc
gut filter_tf -InFile envisat_sgdr_gut_tf.nc -Fg 200km
    -OutFile envisat_sqdr_gut_fg_200.nc
gut import_tf -InFile envisat_cgdr_gut.nc -Ellipse WGS84rev1
    -T mean-tide-OutFile envisat_cqdr_qut_tf.nc
gut filter_tf -InFile envisat_cgdr_gut_tf.nc -Fg 200km
    -OutFile envisat_cgdr_gut_fg_200.nc
gut filter_tf -InFile envisat_sgdr_gut_tf.nc -Fb 200km
    -OutFile envisat_sgdr_gut_fb_200.nc
```

New Output Files: envisat_sgdr_gut_fg_200.nc, envisat_cgdr_gut_fg_200.nc

Results

The results for the full track are shown in Figure 9. The results of both filtering methods produce a clearly improved (smoothed) version of the data, removing the noise and shortwavelength features. The along track mean and rms of the input SGDR data are 0.250 m and 0.671 m respectively. The GUT filtered track has a mean of 0.248 m with an rms of 0.639 m, whilst the GMT filtered track has a mean of 0.243 m and an rms of 0.656 m.

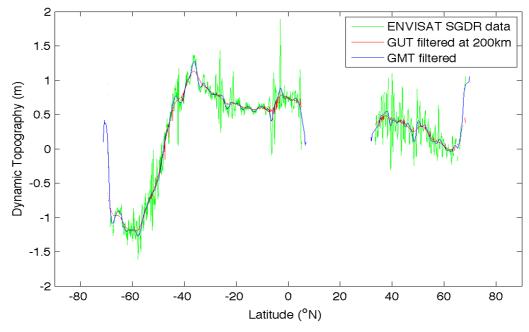


Figure 9 Complete ENVISAT track SLA: raw, filtered by GUT using a 200 km HWHM Gaussian filter, and filtered using GMT with a 400km FWHM Gaussian filter

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In the original version 2 of GUT, there were a number of 'spikes' in the resultant smoothed tracks (see Figure 10). These were caused by a minor error in the coding, when a data point could erroneously drop out of the filter. This has been corrected for v2.1.

Other than these small spikes, GUT deals well with the absent data, either as gaps within the track, or when dealing with a segmented track (Figure 11). There are no spurious endpoint effects, such as seen in GMT.

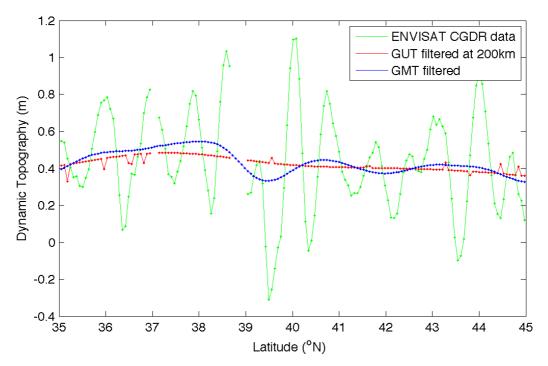


Figure 10 Short section of ENVISAT track SLA: raw, filtered by GUT using a 200 km HWHM Gaussian filter, and filtered using GMT with a 400km FWHM Gaussian filter

However, it is clear that GUT reduces the along-track signal more than GMT. This is particularly true for the sparse (coastal) data case (see Figure 11). At the Southern end of this track, where there are only a few valid data points, GMT generates a continuous curve which passes through the existing data, but GUT produces only short sections, which are approximately 'flat lines'. It could be argued that GMT is, here, producing an unrealistic curve. However, GUT does seem to reduce the variability of the data further that GMT. The weights used within GMT are different to those used by GUT, which explains this effect, but it is not clear if either is 'more correct'.

The additional filter test, carried out with a very simple boxcar filter, produced almost identical results, shown in Figure 12. The only difference here is the small spikes in the GUT filtered data, due to the error mentioned previously. These spikes are not present in data processing using v2.1 of GUT.



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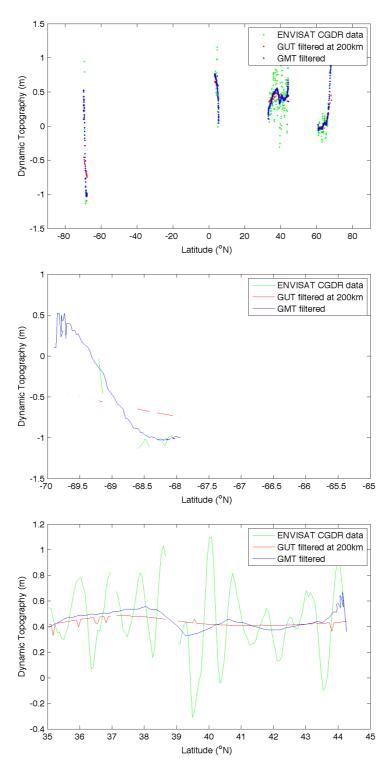


Figure 11 'Coastal' ENVISAT track SLA: raw, filtered by GUT using a 200 km HWHM Gaussian filter, and filtered using GMT with a 400km FWHM Gaussian filter for full pass (top) an for two short sections of the track (middle and bottom)

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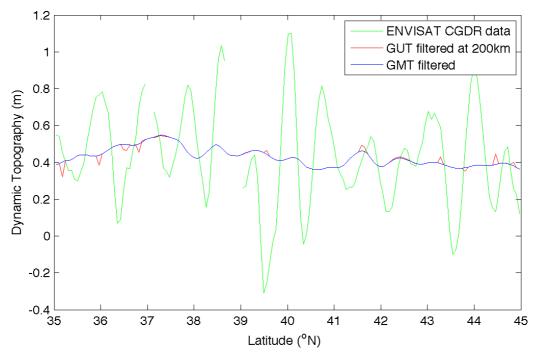


Figure 12 Section of ENVISAT track SLA: raw, filtered by GUT using a 200 km HW boxcar (pillbox) filter, and filtered using GMT with a 400km FWHM boxcar filter

3.3.4 Generate statistics for a limited area

An additional functionality in GUT v2 is the generation of statistics for a specified subregion of a gridded data file. This is particularly useful when interested in sub-regions – e.g. because to concentrate on an area of high or low variability, or away form the coasts. It can also be used to generate zonal averages, although this would take a number of different calls with changing limits. During testing, a coding error was detected that led to longitudes in the range -180 -> 0 being considered as invalid, even for a complete dataset with a longitude grid correctly specified as covering this data range. This has been corrected in v2.1.

This functionality was tested during the testing of anisotropic filtering, when selecting a 'quiet' region in the Pacific.

Results

The statistics generated by GUT were compared with statistics generated within Matlab. The results were identical within the rounding errors of the machines used.



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4 Evaluation of Documentation

The documentation included with the toolbox consists of:

- 1) Installation instructions
- 2) Tutorial
- 3) User Manual
- 4) Workflow definitions accessible from within the toolbox using the --man option and via web pages generated from the workflows.

The installation instructions, provided as a PDF file along with the installation package, provide basic instructions on how each the three separate distribution options (source, windows binary and linux binary) are to be installed. The instructions provide all relevant information to install a functioning version of the software, including the provided workflows and a-priori datasets. The instructions were tested as part of the software test plan, on the tested platforms and provided sufficient information in all cases to install the software given a range of installation requirements.

The tutorial document [AD6] provides:

- Background information on the GOCE mission and data
- Recommendations on the generation of a mean dynamic topography using the toolbox
- Examples of how to use the toolbox for a range of operations, including generation of specialized workflows
- A number of scientific use cases to highlight the potential applications of the toolbox

The tutorial document is the essential introduction to the toolkit, recommended for all users.

The User Manual is a more technical definition of the functionality and implementation of the toolbox. It includes algorithm descriptions and well as full function descriptions and more information on how to build workflows to carry out more advanced procedures within the toolbox. The User Manual is primarily designed as a reference document for those interested in details of the algorithms implemented. It is also a resource for more advanced users, who may be interested in developing specialized workflows or even additional modules. The User Manual has been assessed and is believed to be accurate.

The workflow definitions provide the real-time reference for the toolbox in normal usage. The same information is also accessible through web-formatted version, for browsing in parallel with the toolbox. The reliability of the included workflow information is reliant on the writer of each workflow and has only been confirmed as correct for the workflows in the initial distribution. A minor modification was made to clarify the effect of selecting only a single filter length scale.

During anisotropic filtering testing, a minor error was noted in the documentation for the filter length determination. However, it was confirmed that the code used the correct function, and the documentation has been corrected.

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5 Current Limitations and Suggestions for Enhancement

Most of the limitations recognised in the validation report of GUT v1, and the recommendations for enhancement, have been addressed in the current v2 release. However, there are a number of significant items that were not addressed, and which are reiterated in the current suggestions.

5.1 Interface

5.1.1 Limitation

The toolbox operates through a command line interface. The interface provides access to all the functions, but has clear limitations as a desirable user interface. These include the necessity to have a separate help display, requirement to type and edit commands, to type filenames and to explicitly enter command line options. Whilst familiar to most linux and unix users, relatively few windows or mac users have experience of command line tools, and are far more comfortable with a GUI interface. The unfamiliar interface is probably the major detractor for users when they first try to interact with the toolbox, with some users unsure how to run the program, when not presented with a clickable icon. Although the documentation is there, many users will not look at this and hence never try the software.

5.1.2 Possible future development

A solution to this limitation would be the development of a GUI interface for the toolbox. The interface could allow:

- Allow starting of the application with a clickable icon (even, at the simplest level, to open a terminal window, with a simple instruction printed)
- Building commands from drop down boxes
- 'pop-up' and linked help pages for workflows and options
- selection of input files from folder/directory listings
- Setting user default preferences for workflows
- Direct link to BratDisplay or other data visualisation tool

5.2 Workflow generation and interactive processing

5.2.1 Limitation

This limitation has remained since v1.

Generation of workflows requires manual editing of XML text files. The workflow can be validated using GUT, using the –dot option to generate diagrammatic representation of the workflow to check it operates as expected. However, this is a rather cumbersome method of development, requiring some understanding of the XML structure, which is daunting for inexperienced users. As specialised workflow generation is one of the strengths of the toolbox, this limits the flexibility and usability of the toolbox for many users.



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In addition, there is no way of interaction with workflows during execution, eg to change parameters and investigate a range of parameter options at a particular part of the operation. This kind of functionality would be useful for parameter or diagnostic investigations, such as investigating the dependence of rms field differences on filter length scale.

5.2.2 Possible future development

A solution to this limitation would be the development of a GUI workflow editor, with debug function. Workflows could be halted at defined point, intermediate files generated, and a range of input parameters provided to generate the diagnostics of use.

5.3 **Subsetting**

5.3.1 Limitation

For some of the workflows, the output file may contains a large grid with the majority of the grid values set to NaN, eg when using interpolating a small grid to a larger one using adapt_gf. This is very expensive in terms of graphics when displaying the data. Users may also only wish to display a smaller region, for example when highlighting particular features, and this can most easily be achieved by generating a subset before display.

The toolbox only allows for generation of a 'subset' of the data, using the adapt_gf option, combined with careful use of the options to ensure that the output grid points are identical to those of the subset region. A simple subsetting function would allow extracting the portion of a grid or track within a limited spatial region, without having to know the grid characteristics.

5.3.2 Possible future development

Provide a simple subsetting workflow, which retrieves all grid or track points within specified lat / lon limits, with no interpolation.

Statistics and data reporting 5.4

5.4.1 Limitation

The v2 toolbox allows for simple statistical output for assessment of data generated, enhanced by the option to limit by geographical region, which aids in data assessment and comparison. The statistics provided are limited functions: mean, variance, range and weighted versions. Generation of, eg zonal averages, involves a series of calls to the stats workflow using a range of different subsets.

It is also not possible to interrogate the values of single data points within a data file.

5.4.2 Possible future development

Provide upgraded statistics reporting:

- inclusion of more sophisticated statistics such as zonal or meridional averages.
- Provide data interrogation options retrieval of point-wise data from an input file.

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5.5 Time

5.5.1 Limitation

The v2 implementation of the toolbox allows a basic interpretation of time, allowing a field to be defined as a reference (constant), an instantaneous field or representative of a time period (eg a mean sea surface). Current gravity models are generated for a specific epoch, and some of the spherical harmonic potential coefficients have temporal correction terms. The current version of GUT can retain the information on the epoch of the coefficients, but a GUT format file will not hold the correction terms and is unable to use them to generate output fields for specific epochs.

5.5.2 Possible future development

Develop the GUT format to include time-varying correction terms, specifically for gravity model coefficients.

Calculation of gridded fields, including geoid heights and gravity anomalies, at specific epochs using time-varying correction coefficients from input gravity model coefficients.

5.6 Single Workflows to generate east and north components

5.6.1 Limitation

The current GUT toolbox has a workflow specifically to generate geostrophic velocity, in terms of speed and direction, in a single operation, providing a NetCDF file with both variables. To generate a single file for east and north components, or to generate a single file for east and north vertical deflections, it is still necessary to run two separate GUT workflows (eg gsveast_gf and gsvnorth_gf) and then run the appropriate 'merging' workflow (eg import2_gf).

5.6.2 Possible future development

As it is rare for a user to wish to calculate a single component (east or north) it would be useful to provide a single workflow to calculate geostrophic velocities, with an option to output data as either east and north, or speed and direction, and even an option to ONLY output speed, direction east or north component. Similarly, there could be a single workflow for deflections from the vertical. This would simplify the range of workflows available as well as simplifying the route to generate a single east / north component file.

5.7 Working with multi-parameter files

5.7.1 Limitation

When using functions such as adapt_gf or subtract_gf, only the first parameter, or the defined physical quantity, in a file will be exported. This behaviour is not necessarily as expected, and can lead to overly-complex workflows, eg having generated a single file containing geostrophic speed and direction, the process to generate a subset of this file requires 3 GUT calls – and adapt_gf call for speed, adapt_gf for direction then import2_gf to re-combine these parameters.



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5.7.2 Possible future development

For variables which GUT recognises as vectors, functions that operate on the files, including adapt_gf, subtract_gf, stats_gf, should recognise that both components should be worked on - together, with appropriate warnings and errors if the action is incompatible (eg differencing a file with 2 components from a file containing only one). In the case of stats_gf, it should be possible to select the parameter to generate statistics for using the -PQ option.

5.8 **History attributes**

5.8.1 Limitation

Within GUT v2, the history attribute has been added, to allow the retention of the command used to generate that file. Whilst this is useful, it is still limited, and only provides a single level of history.

5.8.2 Possible future development

Inclusion of additional history attribute(s) within the GUT format NetCDf files, which can retain a longer history of the processing history for a file, including the history of input files used in the processing.

5.9 **Grid adaptation**

5.9.1 Limitation

The grid adaptation routines within GUT v2 offer both a bilinear and a bicubic spline interpolation scheme. This is still only a subset of the available interpolation schemes, which may be preferable in specific circumstances.

5.9.2 Possible future development

Provide alternative grid adaptation options using different interpolation methods.

Given that there are a large number of potential interpolation routines in existence, it is unlikely that the toolbox could ever provide all the possible options users might require. Hence, this may be best developed as an example of a plug-in module, giving a clear demonstration of how users can add their own functions to GUT and incorporate them into workflows.

5.10 Support for Alternative Standard File Formats

5.10.1 Limitation

GUT v2 has enhanced, but still limited, import and export functionality. The recognised formats are NetCDF, gravsoft, GOCE HPF format for import and NetCDF or gravsoft for export. There are a range of alternative, standard formats for gravity data, and simple ascii or binary based formats for gridded data, that it would be useful to be able to import into GUT. Examples include the GRACE and EIGEN spherical harmonic potential format, or

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simple XYZ ascii formatted gridded files. Export is less of a concern, given the availability of the ncdump utility for the GUT output files.

5.10.2 Possible future development

Given the range of potential formats, it will not be possible to allow for input of all formats. However, as part of the tutorial, it could be possible to define a plug-in module, and demonstrate how that could be used, or modified, to read and import a different file format.

5.11 New Workflows for Solid Earth Applications

5.11.1Limitation

GUT v2 is strongly focussed on the needs of the oceanographic community. There is little functionality of specific use to the wider Solid Earth Community, apart from as a tool to 'decode' the GUT format HPF data (potentially to gravsoft format, via netcdf).

5.11.2Possible future development

Workflows have been suggested by the Solid Earth community, for example a simple Bouguer Anomaly calculation. These workflows should be developed and incorporated in the toolbox distribution.

5.12 Speeding Up Calculation for High Degree and Order

5.12.1 Limitation

As was noted, using the toolbox to generate gridded data to high degree and order (greater to 360) and onto high resolution grids (smaller than 5 minute global grids) is not possible using GUT due to the excessive time taken to process.

5.12.2 Possible future development

When working with high DO and/or high spatial resolution gridded output, it may be possible to use alternative processing strategies to speed the files generation. This could be investigated to allow the use of new models in the future.