Data Interpolating Variational Analysis

User Guide

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Conditions of use

Diva is a software developed at the GeoHydrodynamic and Environmental Research (GHER, http://labos.ulg.ac.be/gher/) group at the University of Liège (https://www.uliege.be)) and further developed for SeaDataNet scientific data products in JRA4 activities.

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How to use this guide?

This Diva User Guide aims to cover all the aspects of the methods: the theory (Part I), the two-dimension version (Part II), the climatology production with GODIVA (Part III) and the description of the scripts and the Fortran code (Part IV).

The user who directly wants to perform analysis shall start with Part II, which describes the input files and provides examples of realistic, simple runs. The Diva-demecum (Chapter C) is particularly useful to have a small summary of all the commands and options.

For more theoretical developments, the user is invited to read Part I as well as the corresponding bibliography.

To make easier the reading of the document, different text font and colors are used for different type of files:

- `the files` (ascii or binary),
- `the commands` (which can also be ascii files, but that are executable),
- `the directories`.

Various example files are provided for different situations.

Diva or DIVAnd?

DIVAnd is another software tool developed at GHER and dedicated to the spatial interpolation of in situ data. While the objective is the same as Diva, the method, language and formulation are different.

Note From 2017 on, most of the developments are performed on DIVAnd, Diva is only modified for possible bug corrections.

The table below provides a short summary of the differences. Users interested in DIVAnd are invited to consult the https://github.com/gher-ulg/DIVAnd.jl and to read the article Barth *et al.* (2014).

	Diva	DIVAnd
Language	Fortran, bash	Julia
Dimensions	2	n
Solver	Finite-element, direct (skyline)	Cholesky factorization
Code	https://github.com/gher-ulg/DIVA	https://github.com/gher-ulg/DIVAnd.jl
DOI	doi:10.5281/zenodo.836727	doi:10.5281/zenodo.1303229
Main publication	Troupin *et al.* (2012)	Barth *et al.* (2014)

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- This document:

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  http://www.sciencedirect.com/science/article/pii/S1463500312000790

  BibTeXcode:

```
@ARTICLE{TROUPIN2012bOM,
  author = {C. Troupin and D. Sirjacobs and M. Rixen and
            P. Brasseur and J.-M. Brankart and A. Barth and
            A. Alvera-Azc\'{a}rate and A. Capet and M. Ouberdous and
            F. Lenartz and M.-E. Toussaint and J.-M. Beckers},
  title = {{Generation of analysis and consistent error fields
            using the Data Interpolating Variational Analysis (Diva)}},
  journal = Ocean Modelling,
  year = {2012},
  volume = {52-53},
  pages = {90-101},
  doi = {10.1016/j.ocemod.2012.05.002},
  url = {http://www.sciencedirect.com/science/article/pii/S1463500312000790}
}
```

- the Diva code: we encourage the users to cite the code release they are using in their applications using the corresponding DOI that they can find at https://zenodo.org/record/836727. For instance:
  Version 4.7.1: doi:10.5281/zenodo.836727
  Version 4.6.11: doi:10.5281/zenodo.400970
  ...
  The DOI for all the versions is: doi:10.5281/zenodo.592476

Contents

1 Installation of the software

Diva is a software tool designed to run with any operating system (Microsoft Windows, Linux, Mac OS X). The main steps for the installation are described in this chapter. A more detailed and up-to-date list of instructions is available on the Installation web page of Diva: https://github.com/gher-ulg/DIVA

Warning If you have a previous Diva version running on your system, please make a copy before installing the new version.

Contents

1.1 Requirements

The basic requirements to compile and run Diva are:

1. A command-line interface. With Linux or Mac, the interface is directly available: it is the shell or terminal. With Windows, it is necessary to install a Unix-like environment such as Cygwin (http://www.cygwin.com/).
2. A Fortran 95 compiler with preprocessing `-cpp` possibilities, such as:
   - gfortran (https://gcc.gnu.org/wiki/GFortran),
   - ifort (Intel®, https://software.intel.com/en-us/fortran-compilers),
   - pgf (Portland Group, http://www.pgroup.com/).
3. The netCDF library (http://www.unidata.ucar.edu/software/netcdf/) for Fortran. Note that the library is available in recent versions of the Cygwin installer, but does not properly work in all cases (and you must add the library `nclib=/usr/lib/libnetcdff.dll.a` into the compiling options). When trying to make the Cygwin netCDF library to work, you might need to use

```
[ ~]$ cygcheck netcdfoutput.a
```

to see which libraries are still missing (in our case `sasl`) and therefore to install them with the Cygwin installer.

Other requirements :

1. dos2unix:
   on Linux Ubuntu : sudo apt-get install dos2unix,
   on Cygwin : launch the setup.exe and tick “dos2unix”).
2. bc:
   on Linux Ubuntu : sudo apt-get install bc,
   on Cygwin : launch the setup.exe and tick “bc”.

For a quick visualization of the results, a software tool able to read and display the content of a netCDF file is recommended:

- ncBrowse (http://www.epic.noaa.gov/java/ncBrowse/, a Java application,
- Ncview (http://meteora.ucsd.edu/~pierce/ncview_home_page.html), a visual browser,
- Panoply (http://www.giss.nasa.gov/tools/panoply/, the NASA data viewer for various data formats.

1.2 Download and extraction of the archive

Select a directory on your local disk (here we install in a directory `~/Software/`) where you want install Diva and download the most recent release from https://github.com/gher-ulg/DIVA. You can either download the archive and extract it, or use git if you familiar with the tool.

```
[Software]$ tar -xvf diva-4.7.1.tar.gz
[Software]$ cd diva-4.7.1/
```

The directory tree has the following structure:

```
[diva-4.7.1]$ tree -d -L 2
.
 DIVA3D
    bin
    divastripped
    src
 Example4D
    input
 JRA4
    Climatology
```

- DIVA3D/bin/ contains the executables generated by the code compilation. Pre-compiled executables for various operating systems are provided in the sub-folders.

- DIVA3D/divastripped/ is the main working directory at the 2-D level.
- DIVA3D/src/ contains the Fortran source code. This is where the compilation has to be done.
- JRA4/Climatology/ is the main working directory at the 3-D and 4-D levels.

1.3 Generation of the binaries (executables)

There are two possibilities to obtain the binaries:

1. Compile the source code.
2. Copy the provided binaries.

The second option is provided for cases where the compilation was not possible, mainly because of missing libraries (e.g., netCDF) or Fortran compilers.

1.3.1 Compilation

The compilation is performed in the directory DIVA3D/src/Fortran. There are presently 2 ways to compile the code: through a specific shell script or using the Makefile.

Use the compilation script

Summary:
Edit configuration file divacompile_options and run the shell script divacompileall

```
[Fortran]$ ./divacompileall
```

Detailed explanation:
In the configuration file divacompile_options are prescribed the options for Fortran compiler and libraries.

- If you have already a previous running Diva version and -within it- the file divacompile_options configured according to your system, you can simply copy it to the same place in the new version (diva-4.7.1/DIVA3D/src/Fortran/) before running divacompileall.
- If not proceed as follow:

```
compiler=gfortran
...
DIVA_PARALLEL=1
...
flags='-O3  -cpp   -DDIVAITERATIVE  ' # ' -DDIVABINARYFILESMESH -DDIVABINARYFILES '
```

```
...
flagscalc=' -O3 -cpp   -DDIVAITERATIVE -Wall -fbounds-check'
...
```

If your installation has the nf-config or nc-config commands (installed with the recent netCDF libraries), the compiler and the options for the netCDF library will be detected automatically during the compilation. If you want to check before compilation, type:

```
[~]$ nf-config --fc
gfortran
[~]$ nf-config --flibs
-L/usr/lib -lnetcdff -lnetcdf
```

Check the options of this command by typing nf-config, or visit the web page: http://www.unidata.ucar.edu/software/netcdf/workshops/2011/utilities/Nc-config.html. If you have installed several versions of the netCDF libraries, you might find several nf-config on your system, and each of them may provide you different outputs for the two previous commands. In older versions of netCDF libraries nc-config was used instead of nf-config.

If neither nc-config nor nf-config is installed, you may have to further edit divacompile_options:

```
nclib=/usr/lib/libnetcdff.dll.a
```

Once this is done, run the compilation script:

```
[Fortran] ./divacompileall
```

and check the content of the log file (compilation.log). You should obtain something similar to that:

```
Compilation time:  Wed Jul 15 20:57:28 CEST 2018
compiler:          gfortran
compilation flags: -O3 -frecord-marker=4 -cpp -DDIVAITERATIVE
Calc directory:        1/1 program compiled
Extensions directory: 5/5 programs compiled
Mesh directory:        6/6 programs compiled
NC directory:          8/8 programs compiled
Util directory:        49/49 programs compiled
Pipetest directory:    1/1 program compiled
Stabil directory:      31/31 programs compiled
------------------------------------------------------------
TOTAL:                 101/101 programs compiled
------------------------------------------------------------
Binaries are located in directory:
/home/ctroupin/ULg/Tools/DIVA/DIVA3D/bin
```

Use the Makefile

Edit the file `Makefile` and set the compilers and the compiling flags, then run:

```
[Fortran]$ make
```

1.3.2 Direct copy of pre-compiled binaries

For some releases of the code we also provided pre-compiled binaries. If it is not the case and you have problems to compile the code, we can prepare the binaries for you.

1.4 Run tests

In the main working directory (`diva-4.7.1/DIVA3D/divastripped`), run the available tests: `divatest`, `divabigtest`, `divatest0`, `divatest2`, `divatest3`, `divatesterror` and `test_fit`.

1.4.1 Basic test

`divatest` creates basic input files (see Chapter 6 for details), performs a simple Diva execution, checks if `awk` is appropriate, checks if the pipes are supported in your operating system (O.S.), checks if `dos2unix` is installed. If `divatest` hangs during the pipe test, it means pipes are not supported (as for some gfortran versions) and you can use a `CTRL-C` to exit. The analysis output can be checked using any software for reading NetCDF files. In this case we use ncview (see Chapter 9 for details and installation).

```
[divastripped]$ divatest
...
[divastripped]$ ncview output/ghertonetcdf/results.nc
```

The results you obtain have to be similar to those of Fig. 1.1.

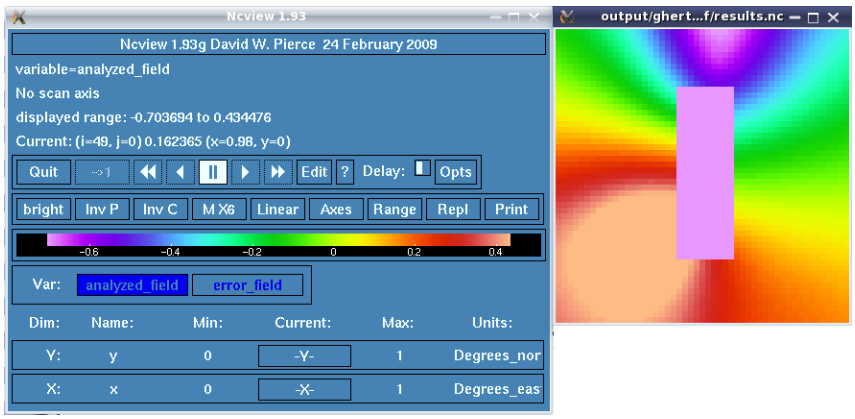


Figure 1.1: Results obtained with `divatest`.

1.4.2 Another basic test

`divatest0` creates basic input files for a fine mesh and a single data point in the center of the domain and runs the analysis. You should obtain the Bessel function with a maximum value close to 0.5.

```
[divastripped]$ divatest0
...
Field value at origin =  0.49961258874045061
```

1.4.3 Large-memory test

`divabigtest` creates input files to simulate a case with a large number of data and a very fine mesh. Again, the results, obtained after a few minutes, are viewable using the command:

```
[divastripped] ncview output/ghertonetcdf/results.nc
```

and should be close to Fig. 1.2.

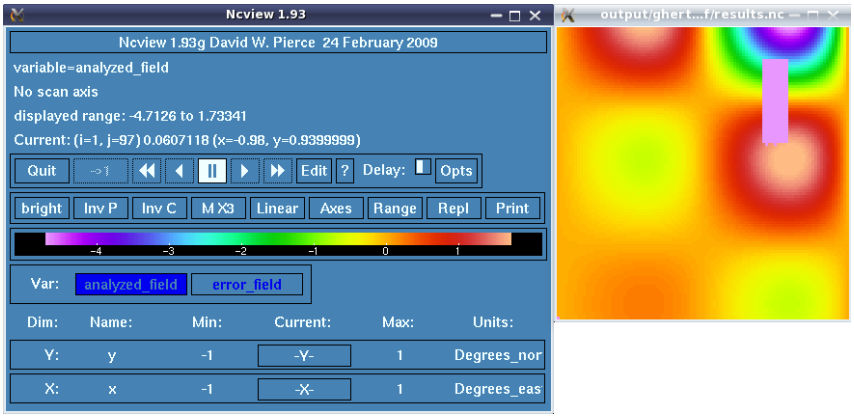


Figure 1.2: Results obtained with `divabigtest`.

Part I

Diva Theory

2 DIVA GENERAL THEORY

This chapter describes the theory behind the Diva interpolation method and compares it with the Optimal Interpolation.

Contents

2.1 Data gridding

The generation of gridded fields from non-uniformly distributed observations (both in space and time) is a frequent concern in geosciences. Similarly to Ooyama (1987), we will refer to an *analysis* or *analysed field* as "*the estimation of a continuous spatial field of a given variable from a set of discrete measurements*". The range of applications is wide, going from model initialization to validation exercises or simple plotting purposes.

Mathematically, gridding consists in determining a field $\varphi(\mathbf{r})$ on a regular grid at positions $\mathbf{r}$, using N_d measurements located in $\mathbf{r_j}, j = 1, \ldots, N_d$ (Fig. 2.1).

In this chapter we consider only two-dimensional cases, but generalization can be done to 3D and even 4D (using "distance" in time, but being aware of autocorrelations as in seasonal signals).

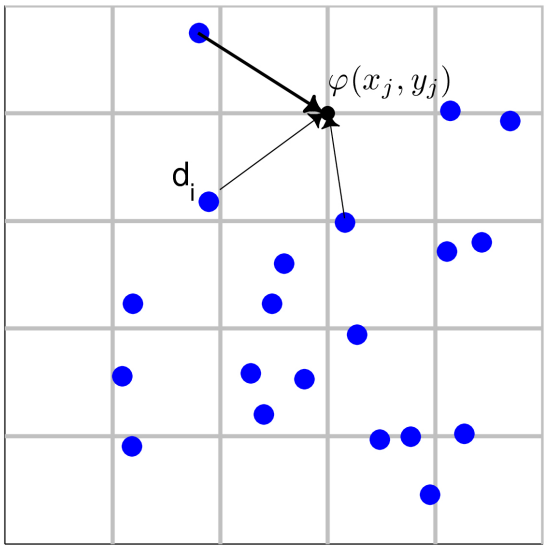


Figure 2.1: Schema of the data gridding: the blue dots indicate data positions, while the nodes of the grid are the points where the field has to be determined.

2.1.1 Interpolation versus approximation

For obtaining a field on a regular grid, two main techniques have to be distinguished:

1. The *interpolation*, which implies a strict passage of the solution through the points of data. Physically, this means that one assumes that there is no error on the data. Among the methods of interpolation, let us mention: the linear, cubic, inverse distance, optimal interpolations, the *kriging*, ...

2. The *approximation* (or *analysis*) provides a solution smoother than the one given by interpolation: in this case, the solution does not necessarily have to contain all the data points. The solution is close to the data points, so its shape is still influenced by the data. This technique allows taking into account errors on data, as well as to treat multiple data with different values at the same location.

Figure 2.2: Interpolation (black line) provides a solution that goes across all the data points, while the approximation (grey line) has only to be "close" to the measurements, but with a relative "smoothness".

2.1.2 Objective versus subjective data analysis methods

In geosciences and in particular in oceanography, it is frequent to have error on the measurements and close data points. Hence the approximation methods are preferred to strict interpolation techniques.

We have to differentiate *subjective* analysis, for which the way the approximation is performed is decided by hand, and *objective* analysis, which is based on predefined mathematical operations. Note that beyond these two kinds of analysis, *data assimilation* uses in addition physical/biochemical dynamic governing equations.

Since data assimilation depends on the region and the model and the subjective analysis is not sufficiently objective, the objective analysis is chosen here.

2.1.3 Background field and anomalies

The field $\varphi(\mathbf{r})$ can be decomposed as the sum of a *background field* φ_b and an anomaly φ':

$$\varphi(\mathbf{r}) = \varphi_b(\mathbf{r}) + \varphi'(\mathbf{r}). \tag{2.1}$$

Instead of working with the data themselves, we will work with the anomalies of these data with respect to the background field. The background field is defined a priori and the anomalies are calculated with respect to this reference field (e.g., climatological average, linear regression, theoretical solution).

The anomalies are assumed to be computed as a linear combination of the data, i.e.,

$$\varphi(\mathbf{r}) = \varphi_b(\mathbf{r}) + \sum_{j=1}^{N_d} w_j \, d_j, \tag{2.2}$$

where d_j is the data anomaly at $\mathbf{r} = \mathbf{r_j}$ and w_j is the relative *weight* of the data j. The weighting functions are the new unknowns to determine: once the background field and the weighting functions are known, the field φ can be computed at any position $\mathbf{r}$, hence gridding is possible.

From here on, we will work with anomaly only and therefore formally use $\varphi_b = 0$.

2.1.4 Noise on data

When measuring a field, there is always an uncertainty on the value obtained (whatever the instrument and the field). *Noise* does not only take into account *instrumental* error (which is generally low), but also:

- the *representativeness* errors, meaning that what one measures is not always what ones intends to analyse):
  e.g., skin temperature, inadequate scales, …
- the *synopticity* errors, occuring when the measurements are assumed to be taken at the same time):
  e.g., data from a cruise (Rixen *et al.*, 2001).

Because of the multiple sources of error, a perfect fit to data is not advised, and the noise on the measurements has to be considered during the analysis.

2.2 The Optimal Interpolation method

Before explaining the core of Diva technique, the main principles of *Optimal interpolation* (OI, von Storch & Zwiers, 1999; Chilès & Delfiner, 1999) are explained. OI is a popular

analysis tool, owing to its ease of use and the error field associated to the analysis (e.g., Shen *et al.*, 1998; Kaplan *et al.*, 2000). The first references of the method are Gandin (1965) and Bretherton *et al.* (1976).

The idea is to minimise the expected error variance of the analysis. This conditions lead to the determination of the weights w_j (2.2), with the assumption that the true anomaly field φ_t is one realization out of a zero mean ensemble.

Note that *Kriging* (Krige, 1951; Matheron, 1963) is an equivalent technique: it uses the same criterion as OI, but with a different mathematical formulation: the weights w_j are chosen from the study of the covariance between the values as a function of the distance between them.

2.2.1 Mathematical formulation

Let us recall previous notations from section 2.1 and introduce some new ones:

φ, the interpolated (or reconstructed) field,
φ_t, the true (unknown) field,
$\mathbf{d}$, the vector containing the N_d data,
$\mathbf{r}$, the vector position.

The principle of OI is to minimize the expected error:

$$e^2(\mathbf{r}) = \overline{[\varphi(\mathbf{r}) - \varphi_t(\mathbf{r})]^2} \tag{2.3}$$

where the bar $\bar{}$ stands for the statistical average.

Replacing the interpolated anomaly field by a linear combination of the data, we have

$$e^2(\mathbf{r}) = \overline{\left[\sum_{i=1}^{N_d} w_i(\mathbf{r}) d_i(\mathbf{r}) - \varphi_t(\mathbf{r})\right]^2}. \tag{2.4}$$

We now have to determine the weights w_i that will minimize (2.4). Let us call $\mathbf{w}(\mathbf{r})$, the vector of size N_d containing the weights applied on the data to interpolate the field at position $\mathbf{r}$. The previous equation is now written as

$$\begin{aligned} e^2(\mathbf{r}) &= \overline{[\mathbf{w}^\mathsf{T}\mathbf{d} - \varphi_t(\mathbf{r})]^2} \\ &= \overline{\varphi_t(\mathbf{r})^2} + \overline{\mathbf{w}^\mathsf{T}\mathbf{d}\mathbf{d}^\mathsf{T}\mathbf{w}} - 2\overline{\varphi_t(\mathbf{r})\mathbf{d}^\mathsf{T}\mathbf{w}} \end{aligned}$$

We define the *covariance matrix*

$$\mathbf{D} = \overline{\mathbf{d}\mathbf{d}^\mathsf{T}},$$

and the covariance of the data with respect to the real field, which is a function of $\mathbf{r}$:

$$\mathbf{g} = \overline{\varphi_t(\mathbf{r})\mathbf{d}}.$$

The expression of the error (2.4) becomes, after some calculation:

$$\begin{aligned} e^2(\mathbf{r}) &= \overline{\varphi_t(\mathbf{r})^2} + \mathbf{w}^\mathsf{T}\mathbf{D}\mathbf{w} - 2\mathbf{g}^\mathsf{T}\mathbf{w} \\ &= \overline{\varphi_t(\mathbf{r})^2} - \mathbf{g}^\mathsf{T}\mathbf{D}^{-1}\mathbf{g} + (\mathbf{w} - \mathbf{D}^{-1}\mathbf{g})^\mathsf{T}\mathbf{D}(\mathbf{w} - \mathbf{D}^{-1}\mathbf{g}) \end{aligned} \tag{2.5}$$

of which the minimum is reached when

$$\mathbf{w} = \mathbf{D}^{-1}\mathbf{g}.$$

The corresponding error value is

$$\min\, e^2(\mathbf{r}) = \overline{\varphi_t(\mathbf{r})^2} - \mathbf{g}^\mathsf{T}\mathbf{D}^{-1}\mathbf{g} \tag{2.6}$$

and the interpolated field is computed as

$$\varphi(\mathbf{r}) = \sum_{i=1}^{N_d} w_i(\mathbf{r}) d_i = \mathbf{g}^\mathsf{T}\mathbf{D}^{-1}\mathbf{d}. \tag{2.7}$$

Derivation of the covariances

To determine the data covariance matrix, $\mathbf{D}$, and the covariance of the data with the real field, $\mathbf{g}$, the following assumptions are generally made:

1. errors ϵ_i on measurements are not correlated, i.e.,

   $$\overline{\epsilon_i \epsilon_j} = \epsilon_i^2 \delta_{ij},$$

   where ϵ_i^2 is the variance of the errors on measurement (i.e., the noise);

2. errors on measurements are not correlated with the real field, i.e.,

   $$\overline{\epsilon_i \varphi_t} = 0.$$

With these assumptions and considering that the data at $\mathbf{r}_i$ is the sum of the true field at $\mathbf{r}_i$ and an error ϵ_i, we deduce:

$$\begin{aligned} D_{ij} &= \overline{\varphi_t(\mathbf{r_i})\varphi_t(\mathbf{r_j})} + \epsilon^2 \delta_{ij} \\ &= \sigma^2\, c(\mathbf{r_i}, \mathbf{r_j}) + \epsilon_i^2 \delta_{ij}, \end{aligned} \tag{2.8}$$

$$\begin{aligned} g_i &= \overline{\varphi_t(\mathbf{r}) d_i}, \\ &= \sigma^2\, c(\mathbf{r}, \mathbf{r_i}), \end{aligned} \tag{2.9}$$

where $c(\mathbf{r}, \mathbf{r_i})$ is the *correlation function* and σ is the *signal* of the data.

In the following, we write $\mathbf{D} = \mathbf{B} + \mathbf{R}$, where matrix $\mathbf{B}$ contains the variance of the true field and $\mathbf{R}$ is the diagonal matrix containing the observational noise.

2.2.2 Drawbacks of OI

There are two main drawbacks when using OI, as detailed in the following paragraphs:

- The numerical cost.
- The specification of the covariances.

As the method requires the inversion of a $N_d \times N_d$ matrix (N_d being the number of data), it is not adapted for situations with large number of observations (number of operations proportional to N_d^3). Moreover the method does not always produce the theoretical optimum, specially when the number of data is not sufficient and the covariances are not correctly specified (e.g., Rixen *et al.*, 2000; Gomis *et al.*, 2001). Some adaptations have been made to the OI scheme to improve the numerical efficiency (e.g., Hartman & Hössjer, 2008; Zhang & Wang, 2010).

The quality of OI (and other gridding techniques) relies on the correct specification of the covariances of the observational error and of the background field. The covariance functions used in OI are not restricted (except that the covariance matrices have to be positive-definite and symmetric), allowing for example correlated observational errors. Yet in most cases, covariances between two points are parametrized by simple expressions, such as a Gaussian function depending on the sole distance between the points, leading to isotropic functions, which are not always well adapted to oceanography. Indeed, wich such functions, the propagation of information through islands and continents is enabled. To circumvent this problem, adaptations of the OI scheme are necessary in order to allow the use of anisotropic functions (e.g., Tandeo *et al.*, 2011).

Finally, although OI provides the best analysis in the sense that it gives the minimum expected error, the method has the drawback of not being fully objective: the covariance of the unknown field, and the standard deviation of observational errors generally have to be chosen subjectively by he user.

2.3 The Variational Inverse Method and its implementation

The Variational Inverse Method (VIM) was initially designed for climatology purposes: in that case, vertical profiles have high vertical resolution and sufficient profiles for all seasons, but have an irregular horizontal coverage (Brasseur *et al.*, 1996). Thus a spatial analysis on horizontal planes is needed.

Relatively large number of data points in each plane penalizes Optimal Interpolation (OI) methods, because these methods require the inversion of a $N_d \times N_d$ matrix (see Tab. 2.2 and eq. 2.6).

This is the reason why VIM resorts to the expertise in efficient finite-element solvers.

Diva stands for *Data-Interpolating Variational Analysis* and is the implementation of VIM. It is designed to solve 2-D differential or variational problems of elliptic type with a finite-element method.

2.3.1 Formulation

We are looking for the field φ which minimizes the variational principle over our domain of interest D:

$$J\left[\varphi\right] = \sum_{j=1}^{Nd} \mu_j \left[d_j - \varphi(x_j, y_j)\right]^2 + \|\varphi\|^2 \tag{2.10}$$

with

$$\|\varphi\| = \int_D (\alpha_2 \boldsymbol{\nabla}\boldsymbol{\nabla}\varphi : \boldsymbol{\nabla}\boldsymbol{\nabla}\varphi + \alpha_1 \boldsymbol{\nabla}\varphi \cdot \boldsymbol{\nabla}\varphi + \alpha_0 \varphi^2)\, dD \tag{2.11}$$

where

- α_0 penalizes the field itself (anomalies),
- α_1 penalizes gradients (no trends),
- α_2 penalizes variability (regularization),
- μ penalizes data-analysis misfits (objective).

Without loss of generality we can chose $\alpha_2 = 1$ (homogeneous function 2.10).

Parameters meaning

Writing Eq. (2.10) and (2.11) in non-dimensional form (with $\frac{1}{L}\tilde{\boldsymbol{\nabla}} = \boldsymbol{\nabla}$, L being a characteristic length of the problem), we have

$$J[\varphi] = \sum_{j=1}^{Nd} \mu[d_j - \varphi(x_j, y_j)]^2 + \int_{\tilde{D}} \left(\frac{1}{L^4} \tilde{\boldsymbol{\nabla}}\tilde{\boldsymbol{\nabla}}\varphi : \tilde{\boldsymbol{\nabla}}\tilde{\boldsymbol{\nabla}}\varphi + \frac{\alpha_1}{L^2} \tilde{\boldsymbol{\nabla}}\varphi \cdot \tilde{\boldsymbol{\nabla}}\varphi + \alpha_0 \varphi^2 \right) L^2\, d\tilde{D} \tag{2.12}$$

and multiplying by L^2:

$$J[\varphi] = \sum_{j=1}^{Nd} \mu L^2[d_j - \varphi(x_j, y_j)]^2 + \int_{\tilde{D}} \left(\tilde{\boldsymbol{\nabla}}\tilde{\boldsymbol{\nabla}}\varphi : \tilde{\boldsymbol{\nabla}}\tilde{\boldsymbol{\nabla}}\varphi + \alpha_1 L^2 \tilde{\boldsymbol{\nabla}}\varphi \cdot \tilde{\boldsymbol{\nabla}}\varphi + \alpha_0 L^4 \varphi^2 \right) d\tilde{D} \tag{2.13}$$

Hence α_0 fixes the length scale over which variations are significant to move the *kernel function* of the norm from one to zero:

$$\alpha_0 L^4 = 1 \tag{2.14}$$

μL^2 fixes the relative weight on data (signal, σ^2) versus regularization (noise, ϵ^2):

$$\mu L^2 = 4\pi \frac{\sigma^2}{\epsilon^2} = 4\pi S/N \tag{2.15}$$

Finally α_1 fixes the influence of gradients:

$$\alpha_1 L^2 = 2\xi \tag{2.16}$$

where $\xi = 1$ if penalization on the gradients is enforced, $\xi = 0$ if no penalization is enforced. ξ is a non-dimensional parameter close to one if the gradients are to be penalized with a similar weight than the second derivatives.

Weights on data

A weight μ_i can be assigned to each data d_i. This weight expresses the confidence you have in a particular data. It is expressed as a function of the signal-to-noise ratio and the correlation length (Brankart & Brasseur., 1996):

$$\mu = \frac{\sigma^2}{\epsilon^2}\frac{4\pi}{L^2} \tag{2.17}$$

when $\xi = 1$. In Diva, the fourth column of the data input file, if present, allows one to apply a different relative weight to each point.

Background field

Normally, interpolation (and extrapolation) works on anomalies with respect to a background field (Eq. 2.1). Diva allows you to work with different background fields:

- no treatment is applied (the data you treat are already anomalies);
- the mean of data is subtracted from the data values;
- the linear regression (plane) is subtracted;
- additional subtracted semi-normed field ($\alpha_0 = 0$ and large L) obtained by two consecutive Diva executions.

In particular when no treatment is applied (with $\alpha_0 > 0$), the minimization forces the analysis toward zero when there are no data points in a distance comparable to L. This is coherent with the idea of an anomaly only.

2.3.2 Resolution by Finite-Element method

The minimization of (2.10) is actually performed by a Finite-Element (FE) method, hence the need for generating a finite-element grid. Because the field to analyse is only defined in the water, the minimization also works only within the contours defining the coastline or more generally, the considered isobath.

Thus the grid generation has to be consistent with the coasts existing in the considered region. The corresponding mathematical problem is referred to the *Constrained Triangulation*.

To solve Eq. (2.10), the real domain is split into a mesh of N_e triangular finite-elements (Fig. 2.3):

$$J[\varphi] = \sum_{e=1}^{N_e} J_e(\varphi_e). \tag{2.18}$$

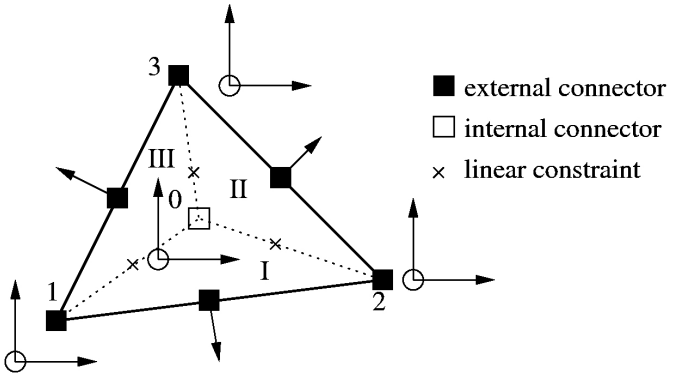


Figure 2.3: Triangular elements used for the mesh. This kind of elements are referred to as "Fraeijs de Veubeke" *elements, see Brasseur (1994) for details. One triangular element is made up of 3 sub-triangles and has a total of 12 degrees of freedom.*

In each element the solution is a combination of shape functions $\mathbf{s}$ (3^{rd} order polynomials) and the continuity between elements is assured by identification of adjacent *connectors*:

$$\varphi_e(\mathbf{r_e}) = \mathbf{q_e}^\mathsf{T}\mathbf{s}(\mathbf{r_e}), \tag{2.19}$$

with $\mathbf{q}$, the connectors (our new unknowns),
$\mathbf{r_e}$, the position in a local coordinate system.

Substituting (2.19) in (2.18) and using the variational principle (2.10), we get

$$J_e(\mathbf{q_e}) = \mathbf{q_e}^\mathsf{T}\mathbf{K_e}\mathbf{q_e} - 2\mathbf{q_e}^\mathsf{T}\mathbf{g_e} + \sum_{i=1}^{N_{d_e}} \mu_i d_i \tag{2.20}$$

where $\mathbf{K_e}$ is the *local stiffness* matrix and
$\mathbf{g}$ is a vector which depends on local data. Matrix $\mathbf{K}$ is decomposed into a norm-related term and a data related term.

On the whole domain, (2.20) reads

$$J(\mathbf{q}) = \mathbf{q}^\mathsf{T}\mathbf{K}\mathbf{q} - 2\mathbf{q_e}^\mathsf{T}\mathbf{g_e} + \sum_{i=1}^{N_d} \mu_i d_i, \tag{2.21}$$

of which the minimum is reached when

$$\mathbf{q} = \mathbf{K}^{-1}\mathbf{g}. \tag{2.22}$$

Matrix $\mathbf{K}$ has a size approximatively proportional to the number of degrees of freedom of the system, but can be very sparse if the elements are properly sorted. In that case the number of operations to invert it is approximatively proportional to the power 5/2 of the number of degrees of freedom.

To map the data on the finite element mesh, a transfer operator $\mathbf{T_2}$ (depending on the shape functions) is applied:

$$\mathbf{g} = \mathbf{T_2}(\mathbf{r})\mathbf{d},$$

and to have the solution at any location inside the domain, another transfer $\mathbf{T_1}$ is applied:

$$\boldsymbol{\varphi}(\mathbf{r}) = \mathbf{T_1}(\mathbf{r})\mathbf{q}.$$

Combining the two previous equations, we obtain the relation between φ, the interpolated field at location $\mathbf{r}$, and the data vector $\mathbf{d}$:

$$\boldsymbol{\varphi} = \mathbf{T_1}(\mathbf{r})\mathbf{K}^{-1}\mathbf{T_2}(\mathbf{r})\mathbf{d}. \tag{2.23}$$

2.3.3 Kernel and correlation function

Kernel functions can be examined by analysing a single point with high signal-to-noise ratio and no background field (Fig. 2.4). In this particular case, we performed an analysis with a point located at the center $(0, 0)$ of a square domain. The correlation length is equal to 1 and the signal-to-noise ratio is taken equal to 1000.

The exact function in an infinite domain is given by

$$K(r) = \left(\frac{r}{L}\right) K_1\left(\frac{r}{L}\right), \tag{2.24}$$

where r is the Euclidean distance,
L is the correlation length and
K_1 is the modified Bessel function (Abramowitz & Stegun, 1964, page 359).

The choice of this correlation model results from the mathematical structure of the variational method (Brasseur *et al.*, 1996).

Figure 2.5 shows both the exact solution (2.24) and the correlation function by a single point analysis. The two curves are close to each other, the differences between the two curves being only due to the boundaries.

In an infinite domain, the correlation function was shown to be proportional to the Kernel of the VIM norm.

The Kernel function can be used to calibrate Diva parameters $(\alpha_0, \alpha_1, \mu)$ so as to fit observed covariance functions. This principle is used by the tool `divafit` which helps one to estimate the correlation length (see Section 7.3.1).

It can also be used for specifying the covariance for error calculations (Chapter 4).

2.3.4 Comparison OI–VIM

Rixen *et al.* (2000) compared the two methods by testing quasi-synoptic salinity data.

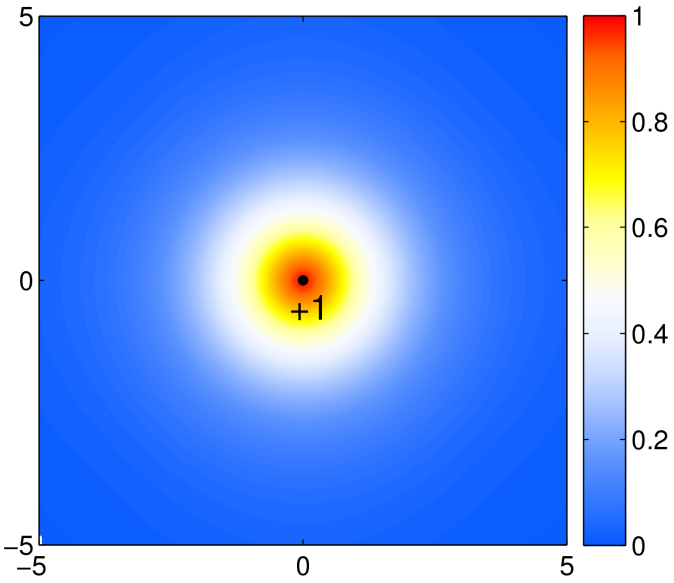


Figure 2.4: Analysis of a single data point with high signal-to-noise ration and no background field.

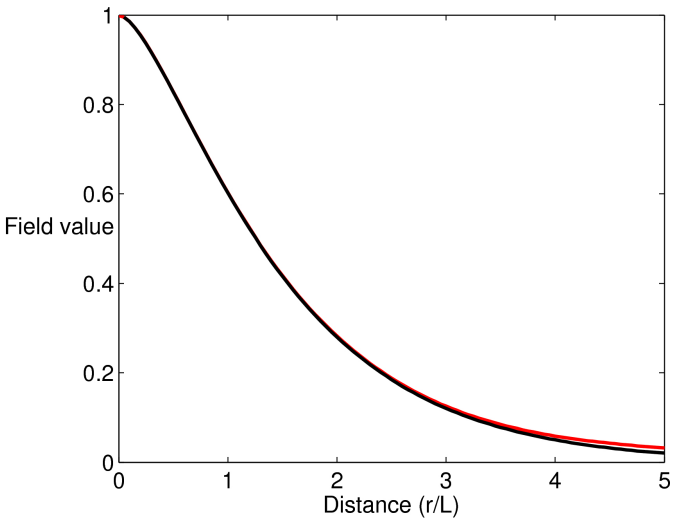


Figure 2.5: The theoretical Kernel function is given in red, while the black curve comes from the analysis of a single point with a unit value.

Results showed that the main differences between OA and VIM occur in coastal areas and around islands ($\mathcal{O}(0.10)$), whereas the differences range from -0.01 to 0.02 within the domain. The same conclusions were drawn when they compared OI and VIM in the case of climatological data set: both fields were nearly identical, except in the vicinity of the coasts (differences of up to 0.1).

A summary of the main characteristics of the two methods is found in Tab. 2.1.

Table 2.1: Statistical equivalence between OI and VIM (from Rixen et al. (2000))

	OI	VIM
Minimization	$e^2(\mathbf{r}) = \overline{[\varphi(\mathbf{r}) - \varphi_t(\mathbf{r})]^2}$	$J[\varphi] = \sum_{i=1}^{N_d} \mu_i [d_i - \phi(\mathbf{r_i})]^2 + \|\varphi\|^2$
Solution	$\varphi(\mathbf{r}) = \mathbf{c}^\mathsf{T}(\mathbf{r})\mathbf{D}^{-1}\mathbf{d}$	$\varphi(\mathbf{r}) = \mathbf{c}^\mathsf{T}(\mathbf{r})\mathbf{D}^{-1}\mathbf{d}$
Data correlation	$[\mathbf{D}]_{ij} = \sigma^2 c(\mathbf{r_i}, \mathbf{r_j}) + \epsilon^2 \delta_{ij}$	$[\mathbf{D}]_{ij} = K(\mathbf{r_i}, \mathbf{r_j}) + (1/\lambda)\delta_{ij}$
Data-field covariance	$[\mathbf{c}]_i = \sigma^2 c(\mathbf{r}, \mathbf{r_i})$	$[\mathbf{c}]_i = K(\mathbf{r}, \mathbf{r_i})$

2.3.5 Comparison between the spatial interpolation methods

Table 2.2 compares characteristics of different spatial interpolation methods:

- the error minimization ($\min(\varepsilon^2)$),
- the extension to 3 dimensions (3-D),
- the multivariate analysis,
- the number of operations per analysis,
- the error estimate ($\varepsilon(\mathbf{r})$),
- *a priori* known parameters,
- the control parameters and
- the treatment of anisotropy.

All the methods compared here are base on a minimisation of the error estimate except the Cressman method (Cressman, 1959). OI and VIM are similar methods: they use the same control parameters and require similar a priori information. To work in 3-D and in multivariate mode, VIM needs a few adaptations. The main difference concerns the number of operations, which is almost independent on the number of data for VIM.

2.4 Additional tools

Diva software is provided with additional tools designed for parameters adjustment, quality control of data and application of physical constraints on the analysis.

Table 2.2: Characteristics of different methods of data analysis. • denote available features in the interpolation method, (•) indicate that the feature is available with some adaptations. $\varepsilon(\mathbf{r})$ is the error estimate, N_d the number of data points, N_a the number of grid points for analysis, N the number of EOFs, L the correlation length and σ^2/ϵ^2 the signal-to-noise ratio.

Method	$\min(\epsilon^2)$	3-D	Multivar	Ops/anal.	$\epsilon(\mathbf{r})$	*a priori*	C.V.	anis.
Cressman		•	•	N_dN_a		$w(r/L)$	(L)	(•)
OI	•	•	•	$N_d^3 + N_dN_a$	•	$c(r/L)$	$L, \sigma^2/\epsilon^2$	(•)
VIM	•	(•)	(•)	$N_a^{5/2}$	•	$K(r/L)$	$L, \sigma^2/\epsilon^2$	(•)
DINEOF	(•)	•	•	$N_a^{5/4}$	•	–	N	•

2.4.1 Automatic estimation of analysis parameters

The correlation length can be estimated, based on the dataset itself. The method performs a least-square fit of the data covariance function with a theoretical function.

The signal-to-noise ratio $\lambda = \sigma^2/\epsilon^2$ is estimated with a Generalized Cross-Validation (GCV). GCV allows estimating global errors and calibration of the analysis parameters.

The tools will be further explained in Chapter 3.

2.4.2 Additional physical constraint

In the base formulation of Diva, the cost function contains a term relative to the regularity of the reconstructed field and a term relative to the proximity to the observations. We will see in Chapter 5 that physics (advection, diffusion, source terms) can be added in the cost function.

2.4.3 Multi-dimensional analysis

In order to perform three-dimension analysis (horizontal coordinates and depth), the solution is to applying successive analysis in horizontal layers, from the deeper to the shallower layer. A set of scripts (`diva3D*`) are designed to perform such analysis in an automatic way.

However, the reconstruction of three-dimensional fields of temperature and salinity by stacking of layers of analysed fields may lead to unstable density fields. An algorithm has been implemented in Diva in order to remove these instabilities.

These topics are addressed in Part III.

2.4.4 DINEOF

Diva is mainly designed to work with in situ data, characterized by a scattered spatial distribution. When dealing with satellite images, the spatial interpolation can be made in a clever way, by using the information contained in the satellite images acquired before in

the same region. This idea is implemented in Data INterpolating Empirical Orthogonal Function (DINEOF; Beckers & Rixen, 2003; Alvera-Azcárate *et al.*, 2005).

This tool is designed to exploit repeated observations with missing data (e.g., a series of collocated satellite images with clouds). For more details about DINEOF, please consult http://modb.oce.ulg.ac.be/mediawiki/index.php/DINEOF and the other references describing the method: Alvera-Azcárate *et al.* (2005, 2007a, 2009); Beckers *et al.* (2006).

3 Determination of analysis parameters

The purpose of this chapter is to describe the tools included in the Diva software and that provide estimates of the analysis parameters: the correlation length L and the signal-to-noise ratio λ. The end of the chapter deals with the automatic quality control of data within the analysis.

Contents

3.1 Determination of the correlation length

The correlation length L gives an indication of the distance over which a given data point influences its neighbourhood (Section 2.3.1). Similarly to other interpolation techniques, it is an essential parameter for obtaining meaningful results. The value of L can be provided a priori by the user, or determined using the data distribution itself, as explained in the next Section.

The method to evaluate L is to fit the theoretical kernel of (2.11) (see Fig. 2.5) to the correlation between data assuming spatial isotropy and homogeneity in correlations. The quality of the fit will depend on the number of data points: a value of L obtained with few data points has to be considered with care.

3.2 Determination of the signal-to-noise ratio

Once the correlation length is determined, the next step is to estimate the signal-to-noise ratio.

3.2.1 Generalities

Let us consider the vector $\mathbf{d}$ containing the N data anomalies. Objective analysis of $\mathbf{d}$ leads to analysed field with minimal expected error variance. The analysis φ^a at any

location $\mathbf{r}$ is given by

$$\varphi^a(\mathbf{r}) = \mathbf{c}(\mathbf{B}+\mathbf{R})^{-1}\mathbf{d} \tag{3.1}$$

where $\mathbf{c}$ is a vector containing the background covariance between the point in which the analysis is to be performed and all data point locations. The optimal interpolation is based on the *background covariance* matrix $\mathbf{B}$ and *error covariance* matrix $\mathbf{R}$ of the data.

Let us call $\tilde{\mathbf{d}}$, the analysis vector at data points. The two vectors $\mathbf{d}$ and $\tilde{\mathbf{d}}$ can be related by the expression:

$$\tilde{\mathbf{d}} = \mathbf{A}\mathbf{d} \tag{3.2}$$

where the matrix $\mathbf{A}$, used to perform the analysis at the data points, is calculated according to

$$\mathbf{A} = \mathbf{B}(\mathbf{B}+\mathbf{R})^{-1}. \tag{3.3}$$

The *data-covariance* matrix is the statistical average $\langle \quad \rangle$ of data products:

$$\left\langle \mathbf{d}\,\mathbf{d}^{\mathsf{T}} \right\rangle = \mathbf{B}+\mathbf{R}, \tag{3.4}$$

where $^{\mathsf{T}}$ it the transposed matrix or vector. For uncorrelated observational errors, error-covariance matrix $\mathbf{R}$ is diagonal, with a variance ϵ_i^2 for point i, *i.e.*

$$\mathbf{R} = \mathrm{diag}(\epsilon_i^2)$$

In that case, we can show that the variance of expected misfit at point i is

$$\left\langle \left(d_i - \tilde{d}_i\right)^2 \right\rangle = \epsilon_i^2(1-A_{ii}). \tag{3.5}$$

In practice covariance matrices are known only imperfectly: their structure is often considered to be fixed, but with imperfectly known amplitude. In other words it is often assumed that

$$\mathbf{B} = \sigma^2\hat{\mathbf{B}}, \tag{3.6a}$$
$$\mathbf{R} = \epsilon^2\hat{\mathbf{R}}, \tag{3.6b}$$
$$\frac{\mathbf{d}^{\mathsf{T}}\mathbf{d}}{N} = \sigma^2+\epsilon^2, \tag{3.6c}$$

where $\hat{}$ matrices are fixed and non-dimensional, while the field variance σ^2 and the error variance ϵ^2 are imperfectly known, but their sum equal to the data variance (assuming that spatial averaging has a similar effect than statistical averaging, the ergodic hypothesis).

By definition of the average error- and field-variance, we have:

$$\frac{1}{N}\sum_{i=1}^{N}\epsilon_i^2 = \frac{1}{N}\text{trace}\,(\mathbf{R}) = \epsilon^2 \quad \Rightarrow \frac{1}{N}\text{trace}\left(\hat{\mathbf{R}}\right) = 1 \tag{3.7}$$

$$\frac{1}{N}\sigma_i^2 = \frac{1}{N}\text{trace}\,(\mathbf{B}) = \sigma^2 \quad \Rightarrow \frac{1}{N}\text{trace}\left(\hat{\mathbf{B}}\right) = 1 \tag{3.8}$$

The unknown parameter that controls the analysis is the ratio of the signal and noise variances, called *signal-to-noise ratio*:

$$\lambda = \frac{\sigma^2}{\epsilon^2}, \tag{3.9}$$

because matrix $\mathbf{A}$ depends only on λ:

$$\mathbf{A}(\lambda) = \hat{\mathbf{B}}(\hat{\mathbf{B}} + \lambda^{-1}\hat{\mathbf{R}})^{-1}. \tag{3.10}$$

Dividing both sides of Eq. (3.6c) by σ^2 and ϵ^2, we also find that

$$\sigma^2 = \frac{\lambda}{1+\lambda}\frac{\mathbf{d}^\mathsf{T}\mathbf{d}}{N}, \tag{3.11}$$

$$\epsilon^2 = \frac{1}{1+\lambda}\frac{\mathbf{d}^\mathsf{T}\mathbf{d}}{N}, \tag{3.12}$$

so that knowing λ we can calculate the signal and noise variances from the data values.

3.2.2 Ordinary Cross Validation (OCV)

The objective is to optimize the parameter λ by searching for its value for which the analysis has a minimal error. For this reason, we need to find a proxy norm that we will be able to minimize. As the difference of the analysis with the true field is not available, we could try to work with the difference of the analysed field at the data points with respect to the original data field:

$$\theta_i^2 = (d_i - \tilde{d}_i)^2. \tag{3.13}$$

If we try to minimize this norm, we will get an infinite signal-to-noise ratio and a perfect data-analysis fit. This is because the analysis at the data point is directly influenced by the corresponding data.

To avoid this inconvenience, the solution is to calculate the difference of the data value with respect to the analysed field in which the data under investigation was not taken into account. This is called the *Ordinary Cross Validation* and is, with a practical trick, implemented in `divacv`. To make this estimate robust, the analysis has to be repeated over a large number of data points, increasing the computing cost, so that OCV is generally too expensive to perform unless a trick as in `divacv` can be used (there the analysis can be done without actually disregarding a data point but by correcting the difference as shown in the next section).

Variants of OCV take out several points at once to calculate error estimates and repeat the exercise several times to make estimates robust. In Diva this options are available in `divacvrand`. A variant is `divacvclasses` in which all data from a given class (e.g. specific year) are set aside and the analysis compared to.

3.2.3 Generalised cross validation (GCV)

According to Craven & Wahba (1978), modifying the error estimate as follows:

$$\hat{\theta}_i^2 = \frac{(d_i - \tilde{d}_i)^2}{(1 - A_{ii})^2}. \tag{3.14}$$

allows one to keep the data during the analysis and will reduce the computing cost. In this formulation, the denominator penalizes more heavily data points in which the analysis is forced to be close the data and accounts therefore for the self-influence of the data point (which is absent in the case of pure cross-validation).

Computation of A_{ii}

When the matrix $\mathbf{A}$ is not explicitly calculated, A_{ii} can be obtained by performing an analysis with a vector $\mathbf{e}_i = (0\,0\ldots 0\,1\,0\ldots 0)$ (zero on all data locations, except at point i, where its value is one). This demands an analysis for every data point in which the estimator is constructed.

The associated computational cost can be reduced by replacing A_{ii} by the average value and assuming:

$$A_{ii} \simeq \frac{1}{N}\mathrm{trace}\,(\mathbf{A})\,. \tag{3.15}$$

To avoid calculating all A_{ii} and summing them up, we can use the following estimate (Girard, 1989):

$$\frac{1}{N}\mathrm{trace}\,(\mathbf{A}) \simeq \frac{\mathbf{z}^\mathsf{T}\mathbf{A}\mathbf{z}}{\mathbf{z}^\mathsf{T}\mathbf{z}} \tag{3.16}$$

where $\mathbf{z}$ is a vector of random variables of zero mean. For robustness, the trace estimate can be repeated several times with different random vectors, averaging of the different estimates. The number of estimates is the parameter provided to the module `GCVFAC` of Diva.

Even if $\mathbf{A}$ is not available, $\mathbf{A}\mathbf{z}$ can be calculated easily by applying the analysis tool to a random vector and retrieve the analysis of this random vector on the data locations. Then the scalar product of the analysis of the random vector with the original random data provides the numerator of (3.16) while the denominator is simply the squared norm of the random vector.

Generalized cross validator

In order to make the error estimator robust, we take the average over all data points and define the *generalized cross validator* as

$$\Theta^2 = \frac{1}{N}\sum_{i=1}^{N}\hat{\theta}_i^2.$$

Assuming temporarily $\epsilon_i^2 = \epsilon^2$, hence having all misfits with the same weight, the generalized cross validator is obtained:

$$\Theta^2 = \frac{\| \mathbf{d} - \tilde{\mathbf{d}} \|^2}{N\left(1 - \frac{1}{N}\text{trace}\,(\mathbf{A})\right)^2} = \frac{\| (\mathbf{I} - \mathbf{A})\mathbf{d} \|^2}{(1/N)\left(\text{trace}\,(\mathbf{I} - \mathbf{A})\right)^2} \tag{3.17}$$

The GCV consists in minimizing Θ^2 by changing the signal-to-noise ratio λ. Θ^2 is a global estimate of the analysis error variance.

In view of (3.5) and (3.17) the expected variance of the noise can also, by assuming a spatial average corresponds to a statistical expectation, be calculated as

$$\epsilon^2 \simeq \Theta^2\left(1 - \frac{1}{N}\text{trace}\,(\mathbf{A})\right) \tag{3.18}$$

When the observational errors are uncorrelated but vary in space, we should replace the residual measure $r = (\mathbf{d} - \tilde{\mathbf{d}})^{\mathsf{T}}(\mathbf{d} - \tilde{\mathbf{d}})$ by

$$r = (\mathbf{d} - \tilde{\mathbf{d}})^{\mathsf{T}}\,\hat{\mathbf{R}}^{-1}\,(\mathbf{d} - \tilde{\mathbf{d}}) \tag{3.19}$$

to take into account the relative noise level.

For a diagonal matrix, we can define weights w_i such that

$$\epsilon_i^2 = \frac{\epsilon^2}{w_i} = \frac{\sigma^2}{\lambda}\frac{1}{w_i} \tag{3.20}$$

Defining the diagonal matrix $\mathbf{W} = \text{diag}(w_i)$, the generalized cross validator then reads:

$$\Theta^2 = \frac{\left(\mathbf{d} - \tilde{\mathbf{d}}\right)^{\mathsf{T}}\mathbf{W}\left(\mathbf{d} - \tilde{\mathbf{d}}\right)}{N\left(1 - \frac{1}{N}\text{trace}\,(\mathbf{A})\right)^2} \tag{3.21}$$

where the weights should, according to (3.7), satisfy

$$\sum_i \frac{1}{w_i} = N. \tag{3.22}$$

The $\tilde{w}_i$ are the values provided as optional fourth column in `data.dat`.

`divacv` uses cross validation with complete calculation of A_{ii}, whereas `divagcv` uses the approximation $A_{ii}N = \text{trace}\,(\mathbf{A})$.

3.3 Quality control of data

Having defined the generalized cross validator, we look for a criterion that will allow the user to reject or accept a given data. Note that this QC is performed based on the analysis itself and shall be preceded by an a priori QC on the data (e.g., range of values, gradients, etc).

3.3.1 Quality criteria

The first possibility is to compare the actual value of the misfit with the expected standard deviation $\left\langle \left(d_i - \tilde{d}_i\right)^2 \right\rangle$, leading to the criterion:

$$|d_i - \tilde{d}_i| > 3\Delta_i^{(1)} \tag{3.23}$$

$$\text{with} \qquad \Delta_i^{(1)} = \epsilon_i \sqrt{1 - A_{ii}}, \tag{3.24}$$

which is the most expensive version if A_{ii} is not explicitly known and must be evaluated by analysis of vectors such as $\mathbf{e}_i = (0\,0\ldots 0\,1\,0\ldots 0)$.

If we replace A_{ii} by its average $\frac{1}{N}\text{trace}\,(\mathbf{A})$, we have a second criterion based on:

$$\Delta_i^{(2)} = \epsilon_i \sqrt{\left(1 - \frac{1}{N}\text{trace}\,(\mathbf{A})\right)}. \tag{3.25}$$

This version requires only a few analysis of a random vector if trace $(\mathbf{A})$ cannot be evaluated explicitly.

Finally, in case the noise is not calculated from Θ^2, another estimate is then, according to (3.18)

$$\Delta_i^{(3)} = \frac{\epsilon_i}{\epsilon}\left(1 - \frac{1}{N}\text{trace}\,(\mathbf{A})\right)\Theta, \tag{3.26}$$

which can be calculated directly from the RMS value of the misfit (or residual) and the generalized cross validator Θ. This version can easily be used simultaneously with test (3.25) using the results of the GCV.

3.3.2 Normalized version

Let us consider the scaled variable s defined as

$$s_i = \frac{d_i - \tilde{d}_i}{\Delta_i}. \tag{3.27}$$

Because we will look for outliers, instead of working with mean values and variances, more robust estimators are the median and *median absolute deviation* (MAD).

A bias in the analysis is likely to exist if $S = \text{median}(s_i)$ is not much smaller than one (the typical values of s should be of the order of one if the misfit estimate is correct on average).

Instead of calculating the standard deviation of s we calculate the median absolute deviation δ defined as

$$\delta = \mathrm{MAD}(s_i) = 1.4826\,\mathrm{median}|s_i - S| \tag{3.28}$$

where the factor 1.4826 is introduced such that for a normal distribution, the MAD is identical to the standard deviation.

Hence we can detect points qualified as outliers if they satisfy the inequality

$$|s_i - S| \geq 3\delta. \tag{3.29}$$

This normalized version of quality control to some extent corrects for inaccurate estimation of the expected misfits Δ.

3.3.3 Implementation in Diva

The overall signal-to-noise ratio λ is calculated as

$$\lambda = \frac{\sigma^2}{\epsilon^2}. \tag{3.30}$$

The relative weights on the data are then defined as

$$\tilde{w}_i = \frac{\mu_i L^2}{4\pi\lambda}. \tag{3.31}$$

To be coherent with the total noise, we should in principle use relative weights (the optional fourth column for data in Diva) on the data that satisfy (3.22).

Hence, defining $\bar{w}$ as

$$\frac{1}{\bar{w}} = \frac{1}{N}\sum_i \frac{1}{\tilde{w}_i}, \tag{3.32}$$

the weights $w_i = \tilde{w}_i/\bar{w}$ are relative weights coherent with the noise.

In this case, we can use (3.21) for the estimator.

In practice, in Diva, the relative weights can be retrieved by $w_i = \mu_i/\bar{\mu}$, where the average $\bar{}$ is a harmonic mean. The minimisation and the optimum for λ are the same, even if the weights provided by the user do not satisfy the condition (3.22). However the interpretation of Θ, ϵ and σ might be different.

Three scripts are available for the QC:

`divaqc`: the most expensive version of QC, based on criterion (3.24).

`divaqcbis`: a quicker version, based on criterion (3.25).

`divaqcter`: based on the RMS value of the misfit and the generalized cross validator Θ, according to criterion (3.26).

Diva GCV practicals

In Diva, the matrix $\mathbf{A}$ is not explicitly constructed, but the product $\mathbf{Ax}$ consists simply in the application of the analysis in data locations.

The value of trace $(\mathbf{A})$ can be evaluated and stored for subsequent quality control by (3.25) and (3.26). For quality control (3.24), A_{ii} must be evaluated by an analysis of the pseudo-data vector $\mathbf{e}_i$ (zeros everywhere except unit value at point i). The analysis can benefit from the LU decomposition already performed for previous analysis.

4 Error computation

This chapter presents the different methods for computing the error field associated to the analysis, as well as the error resulting from the calculation of the integral of a field over a domain.

Contents

4.1 Introduction

The analysis performed with the optimised parameters should have the lowest global error, as measured by (3.21). Nevertheless, the spatial distribution of the error is also of interest for any interpolation or analysis method, since it gives the user an indication of the reliability of the results. The error field is expected to be affected by:

1. the data coverage: the error field is expected to be higher where the data coverage is lower;
2. the noise on the data: the more uncertainties we have on the data, the higher will be the error field.

OI (Sections 2.2) allows the simultaneous derivation of analysis and error fields:

$$e^2(\mathbf{r}) = \sigma^2(\mathbf{r}) - \mathbf{g}(\mathbf{r})^{\mathsf{T}}\mathbf{D}^{-1}\mathbf{g}(\mathbf{r}), \tag{4.1}$$

where σ^2 is the local variance of the background field. This equality highlights that the error is provided by the analysis of a pseudo-data array containing covariances $\mathbf{g}(\mathbf{r})$.

However, in principle, a new analysis has to be performed for each point $\mathbf{r}$ in which the error is requested and then is not adapted for large data sets. On the contrary, the error calculation in Diva is not trivial since the covariance functions are never explicitly specified. We will see in the next sections how Diva computes this error field.

According to the data sets, the type of analysis (with/without dynamical constraints, constant or variable correlation length, …), several error calculation methods are available with Diva.

4.1.1 The poor man's estimate

To circumvent the main problems (unknown covariance function and repeated analysis), Brasseur (1994) estimated the error by analysing a vector of "covariances" with constant σ^2. As all covariances are identical, the error can be assessed in all locations with the same analysis. The advantage is the fast calculation, but the drawback is a systematic underestimation of the actual errors, since the error reduction by the overestimated covariances (4.1) is also overestimated. The poor man's error field is a very efficient way to assess data-coverage and determine the regions where the analysis cannot be trusted.

4.1.2 The clever poor man's estimate

Compared to the poor man's estimate, this approach still analyses a vector of "covariances" with constant σ^2 but reduces the correlation length so that for isolated observations, the resulting error field is almost exact. When data points are closer to each other (typically within the range of the correlation length), then the methods is still to optimistic.

more to come

4.1.3 The hybrid approach

In this approach, Brankart & Brasseur (1998) and Rixen *et al.* (2000) proposed a heuristic statistical error expression for the VIM: in Diva, error fields are calculated by analogy with OI: since analysis in OI is equivalent to analysis with VIM (insofar as the reproducing Kernel of VIM and the covariance function of OI are identical) and since error field of OI equals analysis of covariance fields, error field of VIM equals analysis (by VIM) of covariance fields.

Mathematically, according to the developments of Section 2.2, we have:

$$\text{Solution OI:} \qquad \varphi(\mathbf{r}) = \underbrace{\mathbf{g}(\mathbf{r})^{\mathsf{T}}\mathbf{D}^{-1}}_{(\star)}\ \mathbf{d} \tag{4.2}$$

$$\text{Solution VIM:} \qquad \varphi(\mathbf{r}) = \underbrace{\mathbf{T_1}(\mathbf{r})\mathbf{K}^{-1}\mathbf{T_2}(\mathbf{r})}_{(\star\star)}\ \mathbf{d} \tag{4.3}$$

$$\text{Error OI:} \qquad e^2(\mathbf{r}) = \sigma^2(\mathbf{r}) - \underbrace{\mathbf{g}(\mathbf{r})^{\mathsf{T}}\mathbf{D}^{-1}}_{(\star)}\ \mathbf{g}(\mathbf{r}) \tag{4.4}$$

$$\rightarrow \text{Error VIM:} \qquad e^2(\mathbf{r}) = \sigma^2(\mathbf{r}) - \underbrace{\mathbf{T_1}(\mathbf{r})\mathbf{K}^{-1}\mathbf{T_2}(\mathbf{r})}_{(\star\star)}\ \mathbf{g}(\mathbf{r}) \tag{4.5}$$

In practice, the data input of the analysis tool for an error calculation is a vector containing the covariance of data points ($\mathbf{g}(\mathbf{r})$) with the point in which the error estimate is to be calculated. The covariance vector to be analysed is calculated using the correlation function (or Kernel) $\mathbf{c}$ of an infinite domain in terms of the Bessel function as shown in (2.24):

$$e^2(\mathbf{r}) = \sigma^2(\mathbf{r}) - \sigma^2(\mathbf{r})\underbrace{\mathbf{T_1}(\mathbf{r})\mathbf{K}^{-1}\mathbf{T_2}(\mathbf{r})}_{(\star\star)}\mathbf{c}(\mathbf{r}) \tag{4.6}$$

In an infinite domain, the error calculation is then "exact", while for more complicated domains, it is nearly exact far away from boundaries, provided no anisotropic constraint (advection constraint, variable length scale, boundaries, …) is activated.

Thus for anisotropic cases, the hybrid error field can provide incoherent results. This is what motivated the evaluation of the real covariance function in Diva.

4.1.4 The real covariance method

If we look back at the OI interpretation, we can place a data of value 1 at location $\mathbf{r}$ and compute the analysis $\varphi_1(\mathbf{r}')$ at a location $\mathbf{r}'$:

$$\varphi_1(\mathbf{r}') = \frac{\lambda\hat{B}(\mathbf{r},\mathbf{r}')}{\lambda\hat{B}(\mathbf{r},\mathbf{r}) + \hat{R}(\mathbf{r})}, \tag{4.7}$$

where $\hat{B}(\mathbf{r},\mathbf{r}')$ is the non-dimensional covariance function between points $\mathbf{r}$ and $\mathbf{r}'$, whereas $\hat{R}$ is the normalized observational error variance. Normalization was done respectively by the background variance σ^2 and noise ϵ^2, yielding the signal-to-noise ratio λ previously defined. At the data location itself, we get the analysis

$$\varphi_1(\mathbf{r}) = \frac{\lambda\hat{B}(\mathbf{r},\mathbf{r})}{\lambda\hat{B}(\mathbf{r},\mathbf{r}) + \hat{R}(\mathbf{r})}. \tag{4.8}$$

In terms of interpretation of the covariance function as the kernel of the norm ((2.11)), it is the background covariance that is modified by the anisotropy and not the noise level. Hence, if we put the unit data value with a unit signal-to-noise ratio in $\mathbf{r}$, we directly have

$$\varphi_1(\mathbf{r}') = \frac{\hat{B}(\mathbf{r},\mathbf{r}')}{\hat{B}(\mathbf{r},\mathbf{r}) + 1} \qquad \text{and} \qquad \varphi_1(\mathbf{r}) = \frac{\hat{B}(\mathbf{r},\mathbf{r})}{\hat{B}(\mathbf{r},\mathbf{r}) + 1}. \tag{4.9}$$

The left-hand sides are provided by the Diva application to the unit data point in location $\mathbf{r}$ with unit signal-to-noise ratio and analysed in any desired location $\mathbf{r}'$ and $\mathbf{r}$. From these two values, it is therefore easy to calculate the covariance function $\hat{B}$ inherently used in Diva.

For the error calculation at a point $\mathbf{r}$, we have the following procedure:

1. Put a unit value at $\mathbf{r}$ and perform an analysis with $\lambda = 1$.
2. Save the result at the locations of the original data and of the error-calculation, where the analysis value is
$$\varphi_0 = \frac{\hat{B}(\mathbf{r},\mathbf{r})}{\hat{B}(\mathbf{r},\mathbf{r})+1}, \tag{4.10}$$
3. Calculate the background variance $\hat{B}(\mathbf{r},\mathbf{r})$ at the error-field location:
$$\hat{B}(\mathbf{r},\mathbf{r}) = \frac{\varphi_0}{1-\varphi_0}. \tag{4.11}$$
4. Calculate the covariance $\hat{B}(\mathbf{r},\mathbf{r}_i)$ between the error location and data locations. Since at the data points i located at $\mathbf{r}_i$, Diva application provides
$$\varphi_i = \frac{\hat{B}(\mathbf{r},\mathbf{r}_i)}{\hat{B}(\mathbf{r},\mathbf{r})+1}, \tag{4.12}$$
the covariance $\hat{B}(\mathbf{r},\mathbf{r}_i)$ is obtained as
$$\hat{B}(\mathbf{r},\mathbf{r}_i) = \frac{\varphi_i}{(1-\varphi_0)}. \tag{4.13}$$

Up to the multiplication constant $1/(1-\varphi_0)$, the non-dimensional covariance of a point in position $\mathbf{r}$ with a list of other points can therefore be obtained by putting a unit data value in $\mathbf{r}$ and taking the value of the analysis at the coordinates of the list of points.

To illustrate the procedure, we take a simple case with one point in the center of the domain, and another point near the boundary. Near the boundary, data points influence more easily the analysis because rigidity is reduced (Fig. 4.1). This translates into a larger background variance. Error fields will therefore be larger near boundaries when there are no nearby data.

From there, applying the correction $1/(1-\varphi_0)$, we can use the covariances as input vector for a second Diva execution, so as to perform an analysis of the covariance and getting access to the error of the analysis at the desired location. Indeed, using the equivalence of Diva and OI, if the analysis step applied to a data vector $\mathbf{d}$ is formally written
$$\varphi_a = \mathbf{H}\mathbf{d}, \tag{4.14}$$
then the error is
$$e^2(\mathbf{r}) = \sigma^2\hat{B}(\mathbf{r},\mathbf{r}) - \sigma^2\mathbf{H}\hat{\mathbf{b}}, \tag{4.15}$$
where $\hat{B}(\mathbf{r},\mathbf{r})$ is the local relative background variance (calculated by (4.11)) and $\hat{\mathbf{b}}$ is a vector filled according to (4.13).

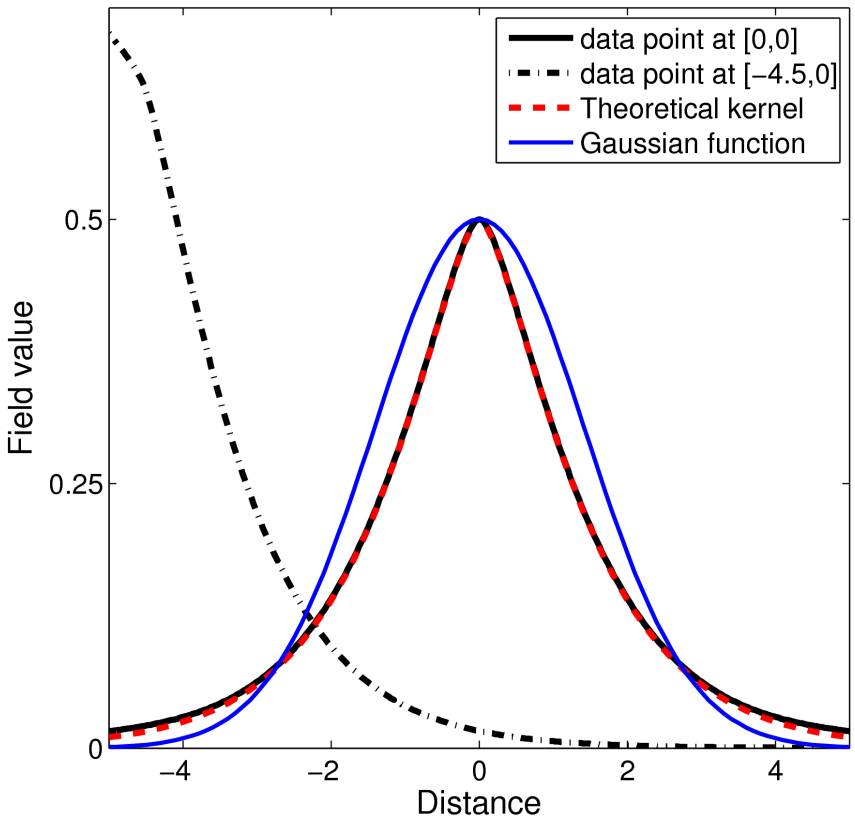


Figure 4.1: Analysis in a square domain $[-5,5] \times [-5,5]$ *with a point at the centre and another at* $(-4.5, 0)$*. The signal-to-noise ratio* $\lambda = 1$ *for both cases. Note the larger analysis value near the boundary, indicating a larger background variance.*

The real covariance method: discussion of background variance

a) Absolute error

b) Errors scaled by B_{ii} When relative errors are demanded, one could divide by $\sigma^2 B_{ii}$;

Discussion The effect of spatially non-uniform B_{ii} is particularly clear at the edge of the finite elements grid. If the boundary is in the open ocean, there is actually no reason to suppose that the background error increases when approaching the artificial boundary and dividing by B_{ii} provides a more natural error estimation so that solution b) should be used.

If near real coasts increased background variance is expected, then the error estimation a) should be used. In such cases, open boundaries should be pushed further away in the numerical finite element grid and the analysis on the regular grid only be done in the region of interest.

4.1.5 The almost exact method

The idea here is to calcule the error exactly in some selected location and than interpolate the error to provide a gridded error field at a reduced cost. The implementation also allows to avoid the need to run a second diva executable by exploiting an expression of the error at data locations by adding pseudo data in well selected locations.

more to come

Background variance

As for the case of the real covariance, one can select to provide the error scaled by B_{ii} or not.

4.2 Usage of methods

The (clever) poor man's error is useful as a first and quick error field during exploration of data. Once analysis parameters such as correlation length are correctly calibrated, outliers eliminated and the analysis considered relevant, a better error calculation should be used.

Calculation of the full covariance function or the almost exact error version for error calculation is recommended when at least one of the following conditions is true:

- Advection constraint is strong.
- Signal-to-noise ratio is high and few data are available near the boundaries.
- ξ (penalizing gradients) is different from 1 and the kernel is not (2.24) any more.

- The correlation length is variable over the domain.

In the aforementioned cases, the assumptions for the hybrid approach are not fulfilled and the use of (4.6) to express the covariance will provide an error field that is not coherent with the analysis. For instance, lower errors can be obtained in regions void of observations.

4.3 Numerical cost

Let us assume that the error is requested at N_c locations (sparse points or regular grid). The error computation with OI (in its original formulation) requires the inversion of a matrix of size $N_d \times N_d$ and the projection of onto the N_c locations. We will now see how it can be done with Diva.

4.3.1 Poor man's estimate

An analysis is performed on a vector filled with constant covariance σ^2. As the vector of covariances is filled with identical values σ^2, the error is assessed for all the N_c locations with the same analysis. Since the matrix to be inverted for the analysis (the stiffness matrix $\mathbf{K}$, (2.22)) is already factorized[1], the additional cost is almost zero because a single analysis is needed.

4.3.2 Hybrid method

Again, the cost is kept low by exploiting the already existing factorization. For each of the N_c locations, matrix-vector operations are needed. Roughly, if the cost of the first analysis is M, the error field calculation requests $MN_c/\sqrt{N_e}$ operations, where N_e is the number of degrees of freedom of the finite-element mesh.

4.3.3 Real covariance function

For each of the N_c points in which the error is to be evaluated, an additional analyse providing the covariance function is needed. If done naively, this would be prohibitive since a new analyse with another data set (the unit data in different locations) normally requests a new matrix inversion.

To save computing time, a nice mathematical property was discovered and exploited: performing an analysis that differs only by one data point from a previous analysis can be performed using an already existing matrix factorization. In this case, the generation of all covariances (always changing only one data point) can be performed with a cost similar to a single error analysis with prescribed mathematical covariance functions.

[1] LU decomposition or factorization: the matrix is written as the product of a lower triangular matrix L and an upper triangular matrix U.

To explain the method, let us suppose that we have constructed and inverted the stiffness matrix $\mathbf{K_0}$ for the same problem without any data point (as explained in Section 2.3.2), $\mathbf{K_0}$ has a component that is related to the smoothness constraint, not to the data). Then, adding a single data point with unit value at location i would demand the solution of

$$\left(\mathbf{K}_0 + \mu_i \mathbf{S}_i \mathbf{S}_i^{\mathsf{T}}\right) \mathbf{q} \;=\; \mu_i \mathbf{S}_i. \tag{4.16}$$

Here, the *Woodbury-Sherman* formula yields

$$\mathbf{q} = \left(\frac{1}{1 + \mu_i \mathbf{S}_i^{\mathsf{T}} \mathbf{K}_0^{-1} \mathbf{S}_i}\right) \mu_i \mathbf{K}_0^{-1} \mathbf{S}_i. \tag{4.17}$$

Since the term in parenthesis is a scalar multiplicative factor, the solution with the data is obtained by analysing this data point with the stiffness matrix $\mathbf{K}_0$ and then multiplying all analyses by $1/(1 + \mu_i \mathbf{S}_i^{\mathsf{T}} \mathbf{K}_0^{-1} \mathbf{S}_i)$. The value of

$$\varphi_0 = \mu_i \mathbf{S}_i^{\mathsf{T}} \mathbf{K}_0^{-1} \mathbf{S}_i \tag{4.18}$$

is actually nothing else than the analysis at the new data location, again using the stiffness matrix $\mathbf{K}_0$. Hence the recipe for calculation of the covariances is now clear:

1. Create and invert once the stiffness matrix $\mathbf{K}_0$ constructed without any data points.
2. For each point for which the covariance is needed:
   (a) Create the elementary charge vector $\mu_i \mathbf{S}_i$.
   (b) Apply the already inverted stiffness matrix $\mathbf{K}_0^{-1}$ and the multiplicative factor of (4.17) to derive the values of φ_0 and φ_i
   (c) Compute the covariances using (4.11) and (4.13).

The efficiency of the method is due to the fact that we remain within the same Diva execution, where the matrix inversion $\mathbf{K}_0^{-1}$ is much less expensive than the initial factorization. Indeed the cost is reduced by a factor $\sqrt{N_e}$, with N_e typically around 10^4-10^5, thus gain is again significant. Each covariance can be stored on disk for later use by the error calculation.

Overall the cost for the full error calculation is now roughly equivalent to twice the hybrid approach, which is a substantial reduction compared to a brute force approach. The only unsolved problem is the storage of the covariance functions if they are calculated before the actual Diva run for the error calculations. This storage will take $N \times N_c$ words when N_c points for error calculations are requested. The intermediate storage can however be avoided by using Unix-pipes between concurrent execution of two Diva cores, one providing the covariance for the other on demand.

4.4 Comparison between the methods

For this application, we employ the same data as in Section 10.1 (salinity measurements in the Mediterranean Sea at a depth of 30 m in July, for the 1980-1990 period). Here, the

error is scaled locally by the local variance of the background field $\hat{B}$, yielding relative errors.

The OI field (Fig. 4.2a) shows the effect of the data coverage on the error magnitude. The relative error lies between 40 and 60% around the regions with a sufficient amount of observations. The largest values ($> 80\%$) occur along the south coasts of the Mediterranean Sea, where almost no data are available for the considered period. This means that the analysis obtained in these areas cannot be taken with much confidence.

The poor man's estimate (Fig. 4.2b) provides an error field with lower values over the whole domain. Where data are available, the error is below 20%, whereas the 80-100% error region is limited to a small zone close to the coast of Libya.

The hybrid method was build by analogy with the OI error estimate (Brankart & Brasseur, 1998). Thus it is expected that the two methods provide comparable results. Indeed, the error field of Figs. 4.2(a) and (c) exhibit a similar spatial distribution. Some discrepancies appear in certain regions: along the Italian coasts (on both side of the Peninsula), in the Alboran Sea, and around Cyprus. These differences are related to the presence of the coasts:

1. As with the analysis, the FE method prevent the information to cross land. Hence the error reduction due to the analysis is lower with the hybrid method than with OI.

2. Close to the coasts, the variance of the background field in Diva is increased, due to the specified boundary conditions.

Finally, the error using the real covariance function (Fig. 4.2d) is also close to the hybrid results. The main differences between the two methods occur in the coastal areas, for instance in the Adriatic Sea or around Cyprus. In these regions, the error is lower when the real covariance is employed, because it allows for the consideration of coastline effects.

The choice of one particular method depends on several factors:

- The size of the output grid.
- The number of analyses to be performed.
- The sources of anisotropies (advection, coastlines).

If the objective is limited to having an indication of the area where the analysed field cannot be trusted, then the poor man's estimate is sufficient. If a more complex error field is to be constructed, a bypass is the reduction of the output grid resolution. This solution is particularly welcome when a large number of analyses ($\mathcal{O}(10^2)$) is required, as it is the case for a climatology (repeated analysis on months and depth levels).

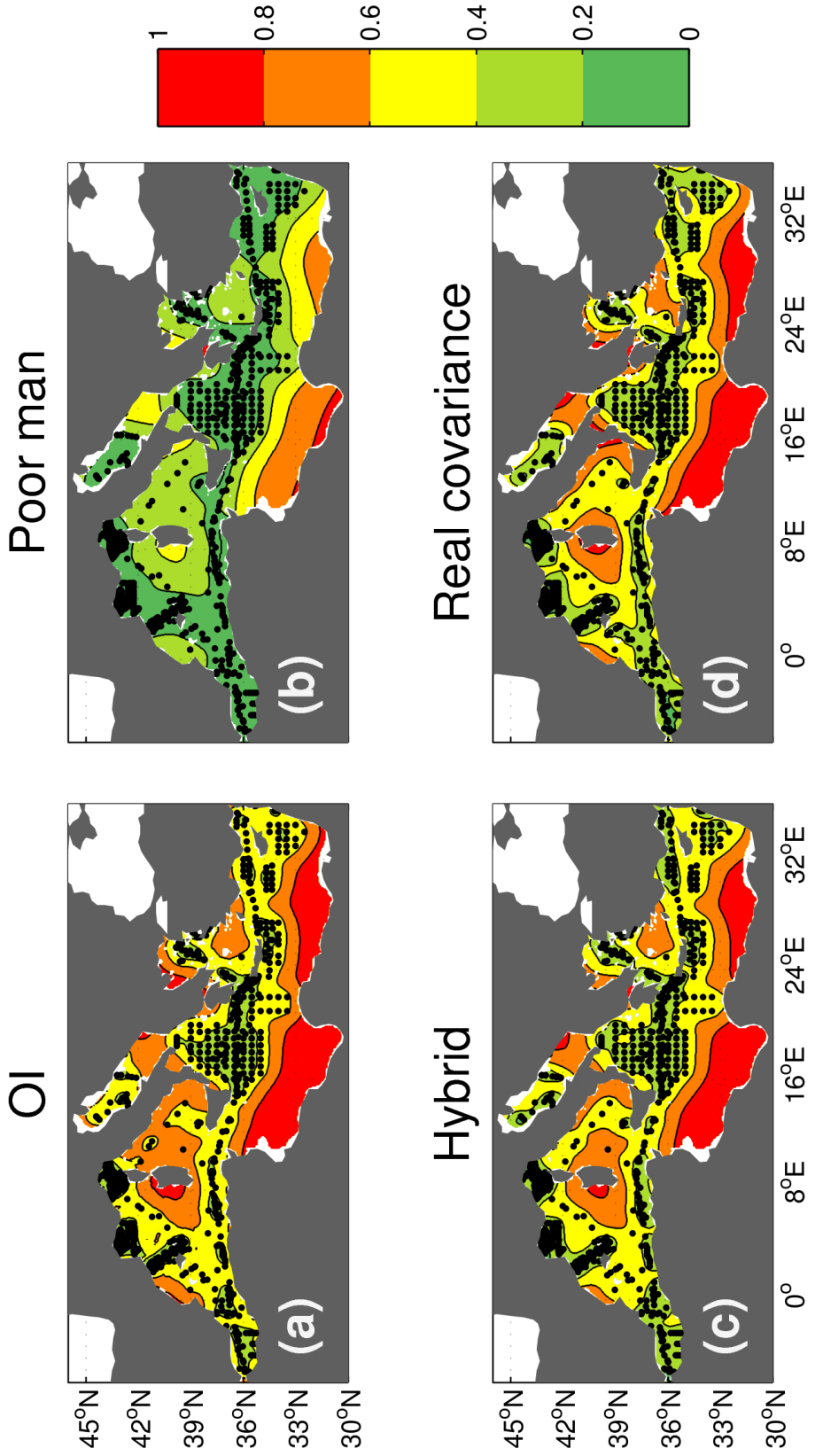


Figure 4.2: Error fields computed using four different methods: (a) OI, (b) poor man's estimate, (c) hybrid and (d) real covariance methods.

4.5 Integrals over (sub-)domains

Very often, we are not only interested in the analysed field itself but also in its integral over the total domain or a sub-domain. If we have the analysis on a sufficiently fine output grid, the integral itself is then just a sum of the values at the grid points covering the integration domain, multiplied by the grid-cell surface.

We do not consider here the additional approximation brought by replacing a continuous integral by a discrete sum. Indeed, generally the output grid is fine compared to the scales of interest and the sum can be considered an "exact" integral. Hence, we will focus on the error on a discrete sum of the analysed field.

An application of this theory is found in Yari *et al.* (2012), where the authors estimated transports through the Strait of Otranto (Adriatic Sea) using Diva and the calculation of integrals.

4.5.1 Theory

Formally, if $\mathbf{x}^a$ is a column vector containing the analysed field values at the grid points defining the integration domain, the weighted sum I over this values is

$$I \;=\; (\mathbf{x}^a)^\mathsf{T}\mathbf{h} \tag{4.19}$$

where $^\mathsf{T}$ stands for the transposed vector or matrix and $\mathbf{h}$ is a column vector of the same size as $\mathbf{x}^a$ but whose components are the weight associated with each integration point. The weight is typically the surface associated with the integration point. For an integration over a uniform grid, the weights can without loss of generality be unit (the surface dimension can be retrieved at the end by global multiplication).

Note that the weights here have nothing to do with the weight on data points for an analysis.

Now the analysis is not exact but has an associated random error ϵ^a with respect to the true field values $\mathbf{x}^t$:

$$\mathbf{x}^a = \mathbf{x}^t + \epsilon^a \tag{4.20}$$

On statistical average (noted $<\quad>$), we suppose the analysis is unbiased and

$$<\mathbf{x}^a>=\mathbf{x}^t \tag{4.21}$$

In order to calculate the error variance on the sum, we calculate the expected square distance with respect to the true sum:

$$\Delta^2 =< \mathbf{h}^\mathsf{T}(\mathbf{x}^a-\mathbf{x}^t)(\mathbf{x}^a-\mathbf{x}^t)^\mathsf{T}\mathbf{h} >= \mathbf{h}^\mathsf{T}\,\mathbf{P}^a\,\mathbf{h} \tag{4.22}$$

where $\mathbf{P}^a =< \epsilon^a\epsilon^{a\mathsf{T}} >$ is the error-covariance matrix of the analysis. We see that the spatial covariances of the analysis-error field are required to calculate the error variance on I. Since this covariance matrix is not diagonal, it is not sufficient to sum up the local error values of the error fields of $\mathbf{x}^a$. The latter sum would limit the double sum of (4.22) to the diagonal terms of $\mathbf{P}^a$.

4.5.2 Implementation

Exploiting the equivalence of Diva and OI, we know that

$$\mathbf{P}^a \;=\; \mathbf{P} - \mathbf{C}^\mathsf{T} \left(\mathbf{B} + \mathbf{R}\right)^{-1} \mathbf{C} \tag{4.23}$$

where $\mathbf{P}$ is the covariance matrix (size $N_g \times N_g$) of the background field between the N_g grid points under consideration, $\mathbf{B}$ the covariance matrix (size $N_d \times N_d$) of the background field between the N_d data points, $\mathbf{C}$ is the covariance matrix (size $N_d \times N_g$) of the background field between the data points and grid points and finally $\mathbf{R}$ is the error covariance matrix (size $N_d \times N_d$) on the data.

We could calculate the covariances matrices involved exactly (as done for the exact error calculation) and then calculate (4.22) but this would be prohibitively expensive if done in a brute force approach. However when done in a clever way it is feasible.

Direct approach

Using (4.23) and (4.22) we can write

$$\Delta^2 = \mathbf{h}^\mathsf{T} \mathbf{P}\, \mathbf{h} - \mathbf{h}^\mathsf{T} \underbrace{\mathbf{C}^\mathsf{T} \left(\mathbf{B} + \mathbf{R}\right)^{-1}}\, \underbrace{\mathbf{C}\, \mathbf{h}} \tag{4.24}$$

The term $\mathbf{C}\,\mathbf{h}$ is readily interpreted as a columns vector containing N_d elements. Element j is the (weighted) sum of the covariances of all integration points with the data point j. The middle term is the analysis operator that provides the analysis on the grid points when providing on input a columns vector of size N_d. Hence the recipe to calculate Δ^2 without explicitly forming the error-covariance matrices is the following:

- Perform a double sum on all covariances between grid points to calculate $\mathbf{h}^\mathsf{T} \mathbf{P}\, \mathbf{h}$.
- For the term to subtract, evaluate it starting from the right: form a pseudo-data vector by summing covariances of all grid points with each data point, analyse it and finally sum up the analysis at the grid points.

All we have to to is to be calculate covariance functions. This can be done with the module `covar` of Diva, which allows one to calculate a series of covariances with a single matrix inversion. Hence the recipe of calculating (4.24) includes a Diva run to calculate covariances (cost roughly equal to an analysis with full error field), followed by a second Diva run to analyse the "data" $\mathbf{C}\,\mathbf{h}$.

Hybrid approach

A simplified version can be used, using to some extend the fact the covariance functions in an infinite domain are known analytically when no advection constraint or variable correlation length is activated. We can indeed introduce an approximation that makes the calculation manageable without calculating the covariances with Diva itself. Instead of using the exact covariances on the background field, we use the covariances we would find

in an infinite domain with constant correlation length and without advection constraint. In this case, we know that the correlation function c between two points is

$$c(r) \;=\; \frac{r}{L} K_1\left(\frac{r}{L}\right) \tag{4.25}$$

where r is the distance between the two points, L the correlation length and K_1 a Bessel function. To get the covariance function we simply have to multiply by the variance σ^2 of the background field.

This way we can estimate Δ^2 by calculating these covariance functions between grid and data points and performing one analysis with Diva.

Inflation approach

A second simplified approach makes even stronger assumptions but shows how we can try to "extrapolate" the error estimated from the sum of the diagonal terms of $\mathbf{P}^a$ to the estimation of the double sum. To do so, we assume that the analysis error has a spatial correlation scale similar to the analysis. This is probably too severe and we will therefore overestimate the integral error. Here we use a continuous formulation to calculate an approximation of Δ noted $\tilde{\Delta}$ by starting from the sum expressed as continuous integral

$$\Delta^2 = \frac{1}{\Delta x^2 \Delta y^2} \int_D \int_D < \epsilon^a(\mathbf{x}) \epsilon^a(\mathbf{x}') > d\mathbf{x}' d\mathbf{x} \tag{4.26}$$

where $\mathbf{x}$ and $\mathbf{x}'$ stand for positions in the domain of integration D. When we suppose the covariance is isotropic and note r the distance between points $\mathbf{x}$ and $\mathbf{x}'$ we have

$$\Delta^2 = \frac{1}{\Delta x^2 \Delta y^2} \int_D \int_D < \epsilon^a(\mathbf{x}) \epsilon^a(\mathbf{x}) > c(r) d\mathbf{x}' d\mathbf{x} \tag{4.27}$$

which we can evaluate in polar coordinates the inner integral expanded to infinity to find an approximate value

$$\tilde{\Delta}^2 = \frac{2\pi}{\Delta x^2 \Delta y^2} \int_D < \epsilon^a(\mathbf{x}) \epsilon^a(\mathbf{x}) > \int_0^\infty r c(r) dr \, d\mathbf{x} \tag{4.28}$$

with the Bessel function for the correlation function c this yields

$$\tilde{\Delta}^2 = \frac{4\pi L^2}{\Delta x^2 \Delta y^2} \int_D < \epsilon^a(\mathbf{x}) \epsilon^a(\mathbf{x}) > d\mathbf{x} \tag{4.29}$$

If we had used the naive approach of neglecting the spatial covariances, the double sum would have been restricted to a simple sum on diagonal and we would calculated the underestimated error

$$\tilde{\tilde{\Delta}}^2 = \frac{1}{\Delta x \Delta y} \int_D < \epsilon^a(\mathbf{x}) \epsilon^a(\mathbf{x}) > d\mathbf{x}. \tag{4.30}$$

Hence we see that we should apply an inflation factor of $\sqrt{\frac{4\pi L^2}{\Delta x \Delta y}}$ on $\tilde{\tilde{\Delta}}$ to get a better estimate of the error standard deviation. In practice this inflation factor is probably a little too high (we assumed the analysis error to have the same correlation length as the analysis while in reality it is generally smaller and we extended one of the integrals to an infinite domain, adding up more errors).

4.5.3 Use

All approaches were implemented into `divaintegral`. If there is a file `./input/integrationpoints.dat`, it will be used. Otherwise it will be created (and put in the `./output`), based on the analysis on the output grid. This files must contain `x,y,val,1,h`. If the file did not exist but was created, it will pass through an execution of `divaintegral`. `divaintegral` can be edited by the user to chose special points for the integration (for example only those points for which the analysis is positive, or points that fall in a given square etc).

When `ispec` is negative, the full covariance calculation will be used. When `ispec` is positive, the hybrid covariance calculation will be used.

When called with the optional argument `-naive`, it also calculates the simple sum of the diagonal term of the analysis error variance. The error field itself is calculated with the methods specified by `ispec`.

```
[divastripped] divaintegral -naive
```

The output files generated are:

- `./output/integral.dat` contains the integral value, the surface of the integration domain and the average value (integral divided by surface).
- `./output/erroronintegral.dat` contains the error standard deviation on the integral, in the same units as the integral.
- `./output/erroronintegralnaive.dat` contains the naive approach summing only the diagonal terms, the inflation factor and the inflated error. Units are the same as the integral.

Units are units of the variable multiplied by the units of x and y of the data and contour file, when no coordinate change is performed or the option `icoordchange = -xscale` was used.

When `icoordchange` is one or two, the surface units of the output are m^2.

Note that the tool is not designed for use with the poor man's error calculation (`ispec`>10, Section 4.1.1).

4.5.4 Interna

- `gridpointlist.a` creates a list of wet points of the analysis grid.

  Input: `fort.20` gridded gher file, `fort.21` corresponding to `GridInfo.dat`.
  Output: `fort.22` list of points with value of analysis on wet points only (`x,y,val,1,1`).

- `erroronintegrals.a` calculates the double sum on background covariance and prepares the pseudo-data (sum of covariances of all grid points with a data point).

  Input: `fort.10` list of grid points for the integral (including third column for value of field), `fort.11` data file, `fort.5` with `scale lc datacol`.
  Output: `fort.14` double sum, `fort.12` pseudo-data vector.

For exact covariance functions,

```
[divastripped] divacalc -pfsum
```

is executed, which allows the use of the full suite of Diva parameters (including for example advection constraint). Internally, as we need the covariance of all integral points with all integral points and data locations, we provide to `divacalc -pfsum` in input "data" which are the integration points and ask in addition values in a list of points (which are the original data location).

5 Additional constraints and detrending

This chapter shows how additional dynamical constraints (advection, diffusion, source, decay) can be added to the cost function that provide the analysed field in Diva. It also describes the *detrending* tool, which allows the extraction of trends from groups.

Contents

5.1 Adding advection to the cost function

Activating an advection constraint on the tracers is done by adding a term to the norm of the field φ (2.11), leading to

$$\tilde{J} = J(\varphi) + \frac{\theta}{U^2 L^2} \int_{\tilde{D}} \left[\mathbf{u} \cdot \tilde{\nabla}\varphi - \frac{\mathcal{A}}{L} \tilde{\nabla} \cdot \tilde{\nabla}\varphi \right]^2 \mathrm{d}\tilde{D} \tag{5.1}$$

where U and L are characteristic velocity and length scales, respectively. We recognize a dimensionless version of stationary advection-diffusion equation

$$\mathbf{u} \cdot \nabla\varphi \;=\; \mathcal{A}\, \nabla \cdot \nabla\varphi \tag{5.2}$$

The parameter θ allows one to adapt the weight of the additional second term, in which we recognize a stationary advection-diffusion equation. The physical meaning of the term $\mathbf{u} \cdot \tilde{\nabla}\varphi$ is simple: when the velocity is nearly parallel to the gradient, the product has a large value and is thus penalized. Then for a strong constraint ($\theta \gg 1$) we enforce the analysis to align with velocity.

In general we can assume $\mathcal{A} \leq UL$, in other words, we work at relatively high *Reynolds numbers* [1]. Otherwise for dominant diffusion, the term just adds another isotropic filtering effect, already included in the regularization term (Eq. 2.11). Hence the additional term is really interesting only for situations dominated by advection, with $\mathcal{A} \leq UL$. In this case, the scaling is such that for $\theta \approx 1$, the advection constraint has a similar importance with respect to the regularization term.

The velocity scale U is calculated from the provided $\mathbf{u} = (u, v)$ field.

Note that when using the advection constraint, the correlation length provided by `divafit` should be decreased since the advection constraint implicitly increases correlation length along currents.

The solution is expanded in terms of so-called connector values (typically values at the nodes of a finite element mesh, and in the present case, also normal derivatives to interfaces) and shape functions over each element (Section 2.3.2). This allows the computation of the solution at any desired location, knowing the connector values.

The connector values themselves are found as the solution of the minimization process:

$$(\mathbf{K}_s + \mathbf{K}_d)\,\mathbf{q} = \mathbf{g} \tag{5.3}$$

The stiffness matrix $\mathbf{K} = \mathbf{K}_s + \mathbf{K}_d$ is composed by the different terms related to the derivatives ($\mathbf{K}_s$) and a final term related to the location of data:

$$\mathbf{K}_d = \sum_{i=1}^{N_d} \mu_i \mathbf{S}_i \mathbf{S}_i^{\mathsf{T}} \tag{5.4}$$

where $\mathbf{S}_i$ is a column vector containing the shape functions associated with a data point i. This vector has zeros everywhere, except for all connectors of the element in which the data point lies.

Similarly, the data value d_i come into the formulation by a projection of the data onto the charge vector of the connectors

$$\mathbf{g}_i = \mu_i \mathbf{S}_i d_i \tag{5.5}$$

and the total charge vector is the sum of the individual ones.

When a constraint is added, in the original version, the stiffness matrix is augmented by components for each element Ω which are computed

$$\int_\Omega \left(u\frac{\partial s_i}{\partial x} + v\frac{\partial s_i}{\partial y} - \mathcal{A}\frac{\partial^2 s_i}{\partial x^2} - \mathcal{A}\frac{\partial^2 s_i}{\partial y^2} \right) \left(u\frac{\partial s_j}{\partial x} + v\frac{\partial s_j}{\partial y} - \mathcal{A}\frac{\partial^2 s_j}{\partial x^2} - \mathcal{A}\frac{\partial^2 s_j}{\partial y^2} \right) \mathrm{d}\Omega \tag{5.6}$$

where s_i are the shape functions of the element

5.1.1 Advection alone

Figure 5.1 shows an example of a single data point located at $(0.7, 60)$ with unit value in a solid rotation (centred in $(0, 60)$). In the absence of diffusion, up and downwind are identical (covariance counts).

[1] The Reynolds number measures the ratio of the inertial effects over the viscosity effects

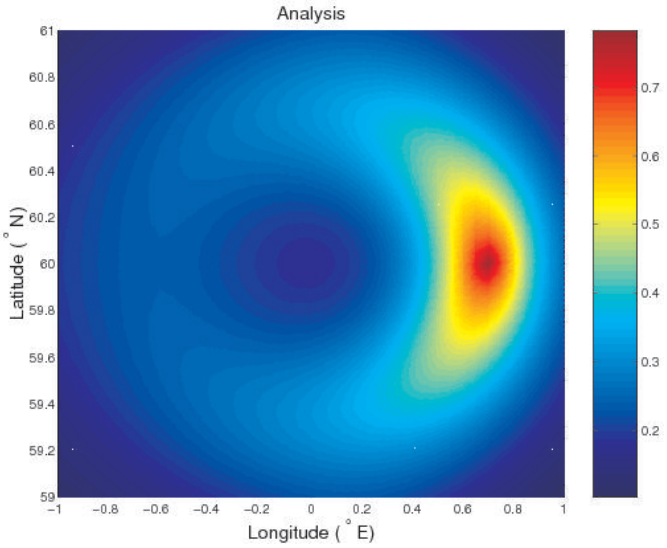


Figure 5.1: Single data point with unit value in a solid rotation.

Without advection (Fig. 5.2), the across velocity scale remains and isotropy is recovered (except for boundary effect on the right side).

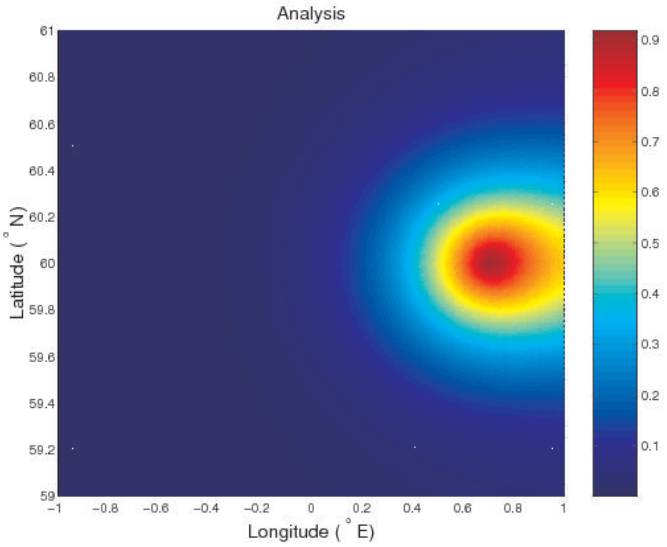


Figure 5.2: Same as Fig. 5.1, but without advection.

To decrease the cross-frontal scale, we must decrease L but add advection to keep along-current scale larger (Fig. 5.3).

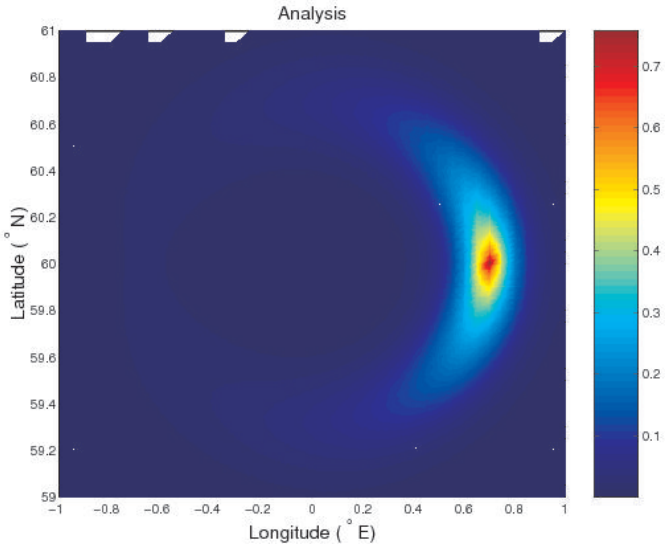


Figure 5.3: Same as Fig. 5.1, but with smaller length scale.

Adding advection without decreasing L increases correlation length along-front and keeps cross-front correlation length.

5.1.2 Advection and diffusion

Adding diffusion makes possible the distinction between up and downwind direction (Fig. 5.4): in this case, higher values are found upwind of the data location: this is natural, because the data is observed and Diva tries to infer the field that explains the sample. This requests higher values upwind (because downwind values decrease).

Because of the square in the formulation, to change the flow direction you can simply change the sign of the diffusion coefficient or change the sign of the velocity components (Fig. 5.5).

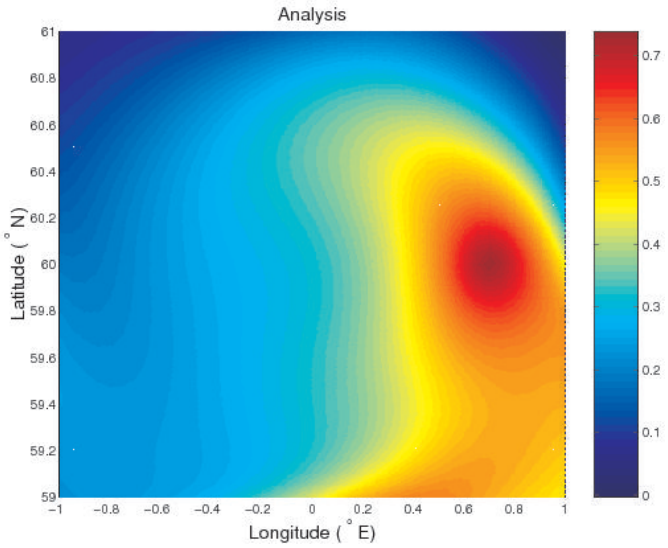


Figure 5.4: Single data point with anti-clockwise rotation and with diffusion.

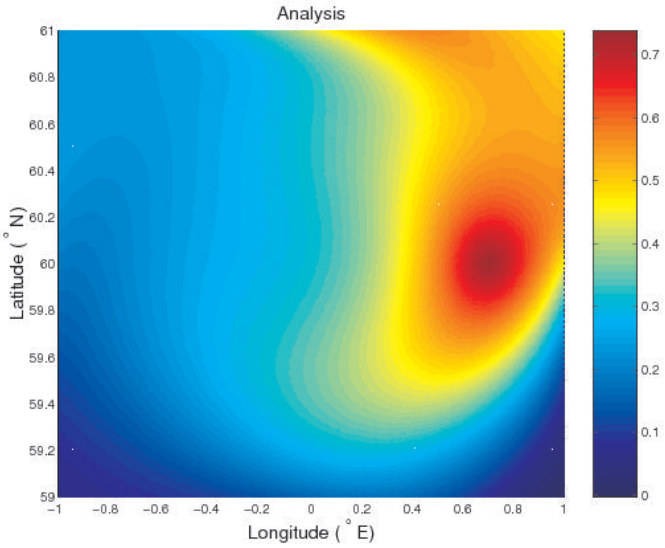


Figure 5.5: Single data point with clockwise rotation and with diffusion.

5.1.3 Generalization

Zero diffusion simply leads to correlations that are increased in the direction of the vector $\mathbf{u}$ (or decreased in the perpendicular direction if the global L is increased simultaneously).

The vector $\mathbf{u}$ does not need to be a velocity in this case, but can be any vector indicating the direction in which correlation is to be increased. Hence it could be for example, topography gradients rotated by 90 degrees or density gradients rotated by 90 degrees if we respectively assume across depth-contour movements are more difficult (and hence data correlation decreased) or across frontal movements more difficult (and hence correlation length across fronts decreased). This idea is implemented in `divaUVtopo` which generates a pseudo velocity field along isobaths.

The advection constraint therefore allows any known anisotropy in the correlations to be included into the analysis. We notice that the vector field does not need to be divergence free.

5.2 Adding linear sink(s) and local source(s)

With the more complete equation

$$\mathbf{u}\cdot\nabla\varphi \;=\; \sum_j \mathcal{Q}_j\delta(\mathbf{r}-\mathbf{r}_j) \;-\gamma\varphi \;+\mathcal{A}\nabla\cdot\nabla\varphi, \tag{5.7}$$

we augment the cost function as

$$\tilde{J} = \tilde{J}_1(\varphi) + \theta\int_{\tilde{D}}\left[\mathbf{u}\cdot\tilde{\nabla}\varphi - \frac{1}{Re}\tilde{\nabla}\cdot\tilde{\nabla}\varphi + \gamma\frac{L}{U}\varphi - \sum_j \mathcal{Q}_j\frac{L}{U}\delta(\mathbf{r}-\mathbf{r}_j)\right]^2 \mathrm{d}\tilde{D}. \tag{5.8}$$

5.2.1 Implementation

$\mathbf{K}_s$ is easily modified by adding the decay term during the calculation of the constraint:

$$\int_\Omega \left(u\frac{\partial s_i}{\partial x} + v\frac{\partial s_i}{\partial y} - \mathcal{A}\frac{\partial^2 s_i}{\partial x^2} - \mathcal{A}\frac{\partial^2 s_i}{\partial y^2} + \gamma s_i \right) \left(u\frac{\partial s_j}{\partial x} + v\frac{\partial s_j}{\partial y} - \mathcal{A}\frac{\partial^2 s_j}{\partial x^2} - \mathcal{A}\frac{\partial^2 s_j}{\partial y^2} + \gamma s_j \right) \mathrm{d}\Omega.$$

The source is a little bit more complicated : each source has a contribution to the charge vector $\mathbf{g}$ of the type

$$2\int_\Omega \left(u\frac{\partial s_i}{\partial x} + v\frac{\partial s_i}{\partial y} - \mathcal{A}\frac{\partial^2 s_i}{\partial x^2} - \mathcal{A}\frac{\partial^2 s_i}{\partial y^2} + \gamma s_i \right) \frac{\mathcal{Q}}{\Omega}\mathrm{d}\Omega \tag{5.9}$$

where $\mathcal{Q}$ is taken constant over the sub-element for simplicity (otherwise we need to calculate the derivatives at the source location instead at the gauss integration points where we know them already).

- Each source (unit= unit of tracer by unit time), is spread over sub-element in which source is found.
- Source file `sources.dat` similar to data file. Read in a similar way and sources sorted in a similar way also (which needed some adaptations)
- Files modified `solver.f constr.f divainc.h datapr.f divacalc`
- File added: `sourcepr.f`
- `constraint.dat` can now contain a third optional parameter which is γ.

Only two possibilities for coordinates and units:

- user coordinates (`icoordchange=0`): velocity (L/T), decay rate (1/T), diffusion (L^2/T) and decay (1/T) and coordinates (L) must have same units. Source has variable unit over time dimension;
- coordinates are degrees and are transformed to km (`icoordchange=1`): velocity must be in m/s, diffusion in m^2/s, decay in 1/s and source in "variable units"/s

Other limitations:

- With decay or source activated, `ireg` should be zero (but is not checked).
- Poor man error field is really bad for these cases.

5.2.2 Example

5.3 Detrending data by defining groups and classes

When analysing climatological data, one is very often faced with data sets that have heterogeneous coverage in time and/or in space. This can lead to misinterpretations of the analysis, if for example there have been much more measurements during a specially warm year than during other years. It is also not uncommon that there are much less cruise data sets in stormy periods than in calm periods.

Here we present a method to deal with such problems by defining *classes* and *groups*.

A *group* is simply one way of subdividing the data into different members. For example a group can be based on years and the classes are 1995, 1996, 1997 if we are looking at this period. Another group could be based on seasons and classes could be winter, spring, summer and autumn.

5.3.1 Theory

In the functional to be minimised by Diva, there is a data-analysis misfit term :

$$\sum_{i=1}^{N_d} = \mu_i \left[d_i - \varphi(x_i, y_i)\right]^2 \tag{5.10}$$

where μ_i is the data weight on data d_i found in location x_i, y_i. The solution of the minimisation is the analysed field $\varphi(x, y)$.

If we define one group, each data point is in one and only one class C_j of this group. Hence when calculating the misfit in the minimisation part of Diva, we include now an (unknown) trend value for each class ($d_{C_1}, d_{C_2} \ldots$):

$$\sum_{i \in C_1} \mu_i \left[d_i - d_{C_1} - \varphi(x_i, y_i)\right]^2 + \sum_{i \in C_2} \mu_i \left[d_i - d_{C_2} - \varphi(x_i, y_i)\right]^2 + ... \tag{5.11}$$

If we assume we know the function $\varphi(x, y)$, minimisation with respect to each of the unknowns d_{C_j} yields

$$d_{C_1} \;=\; \frac{\sum_{i \in C_1} \mu_i \left[d_i - \varphi(x_i, y_i)\right]}{\sum_{i \in C_1} \mu_i} \tag{5.12}$$

and similarly for the other classes. Hence we see that the trend for each class is the weighted misfit of the class with respect to the overall analysis. The problem is of course that φ is not known since it is also the result of the minimisation process. However, we can iterate and start with an analysis without detrending. Then, using the field of φ, we can calculate a first guess of the trends in each group and subtract if from the original data. Then a new analysis can be performed, the trends recalculated and so on until convergence.

5.3.2 Implementation

Here we generalize by allowing several groups of classes.

The detrending is done hierarchically:

1. Trends for the first group are calculated and removed from the data.
2. The second group is treated and so on.
3. Once the data has been detrended, a new diva analysis is performed.
4. With the new analysis, the data-analysis misfit (or residual) can be reused to calculate better estimates of the trends.

This loop is repeated a predefined number of times.

5.3.3 Generalizations

We can further add regularization constraints on the calculated trends. For example, if there a few data available for estimating the trend of class C_j, we should be not be too confident on the trend and rather perform a standard analysis (i.e. reducing the value of d_{C_j}). We can modify the cost function associated with data in class C_j as follows

$$\sum_{i \in C_j} \mu_i \left[d_i - d_{C_j} - \varphi(x_i, y_i) \right]^2 + \alpha_j (d_{C_j})^2 \tag{5.13}$$

where the coefficient α_j regularizes the trend amplitude and

$$d_{C_1} \;=\; \frac{\sum_{i \in C_1} \mu_i \left[d_i - \varphi(x_i, y_i) \right]}{\sum_{i \in C_1} \mu_i + \alpha_i} \tag{5.14}$$

If N_j is the number of points with non-zero weights, we can define

$$\bar{\mu}_j = \frac{1}{N_j} \sum_{i \in C_j} \mu_i \tag{5.15}$$

and a proposed scaling for regularization constants is

$$\alpha_j = \bar{\mu}_j \sqrt{N_j}. \tag{5.16}$$

This has been implemented.

If the detrending is included in a 3-D loop, with the same groups and classes defined in each layer, we can further request that the values of the trends in a given layer are not too far from those in the surrounding layers and modify the norm as

$$\sum_{i \in C_j} \mu_i \left[d_i - d_{C_j} - \varphi(x_i, y_i) \right]^2 + \alpha_j (d_{C_j})^2 + \beta^+ (d^+_{C_j} - d_{C_j})^2 + \beta^- (d^-_{C_j} - d_{C_j})^2 \tag{5.17}$$

where the coefficient β_j^* regularize the trend differences between layers and where $^+$ refers to the value in the layer above and $^-$ to the layer below. Obviously, the solution of this problem will involve tridiagonal solvers. For the lowest and uppermost layer, we can simply assume a zero gradient for the trends.

Similarly, the β can be scaled based on the two layers involved

$$\beta_j^+ = \frac{(\bar{\mu}_j^+ N_j^+ + \bar{\mu}_j N_j)}{(N_j^+ + N_j)} \tag{5.18}$$

This regularisation between layers is not yet implemented. Either done at 3-D level or simply allow iterative 3-D filtering as now but with weights β as described here !

5.3.4 Use

Simply provide `./input/data.dat` with additional fifth, sixth …columns. If you do not want to use variable data weight, column 4 must contain the value of 1. Column 5, 6, …contain the information in which class the data point falls. Classes must be numbered starting with 1.

Example

- Column 5 contains value 1 for a data point of the year 1975, 2 for 1976, 3 for 1977 and so on.
- Column 6 contains 1 for a data corresponding to month 01-03, 2 for the month 04-06 and so on.
- Column 7 contains 1 for day values, 2 for night values.
- Column 8 contains 1 for points that have a density below 1025 kg/m^3, 2 for points that have a density above it.

Execute `divadetrend ngroups [niterations]`. The parameter `ngroups` specifies that the first `ngroups` will be used for the detrending. (You might create for example 5 groups and try with detrending on the first one only using `divadetrend 1`). The optional parameter `niterations` tells how many iterations are to be performed for the detrending. Default value is 10 iterations.

Outputs

`./output/rmsmisfit.dat` contains the evolution during the iterations of the misfit (after detrending). It should decrease if the detrending works well. `trends.all.1.dat` deals with group 1 and contains on column 1 the class number and on columns 2 the final trend value associated with it. Columns 3 and 4 correspond to the next to last iteration and the last columns to the first iteration.

`divagnu` produces plots for the trend in each group.

Notes:

- Presently you can define at maximum 5 groups with each group having 50 classes (members). You can increase these limits by editing and compiling `src/Fortran/detrend.f`
- It is assumed that the mesh already exists, otherwise execute `divamesh` before.

Additional options

If you provide file `detrend.order` in `./input/`, then the columns for detrending will be taken in the order specified in the file.

Example if `detrend.order` contains: `8 5 7 6`
and we call `divadetrend 3`, columns `8 5 7` will be used in this order for detrending. If there is no file `detrend.order`, then `divadetrend 3` will use 5 6 7 in this order.

(file `detrend.order` or default order is written in `fort.56` in `divawork` during execution)

5.3.5 Example

The example located in `Examples/Trends/` contains data sampled from a spatial pattern (sin-cosine structure) over which was added:

- a seasonal cycle,
- a daily cycle and
- inter-annual variations.

Groups are years, month and hours. Matlab file `pseudodata.m` can be used to generated such a data file. The comparison between analysed field without and with detrending option is shown in Fig. 5.6: on the left-hand side, the sin-cosine structure is visible, but perturbed by the various cycles superimposed on it. After the detrending, the structure is perfectly recovered.

Along with the field without trend, the `divadetrend` tool also provides the trend for each group (Fig. 5.7).

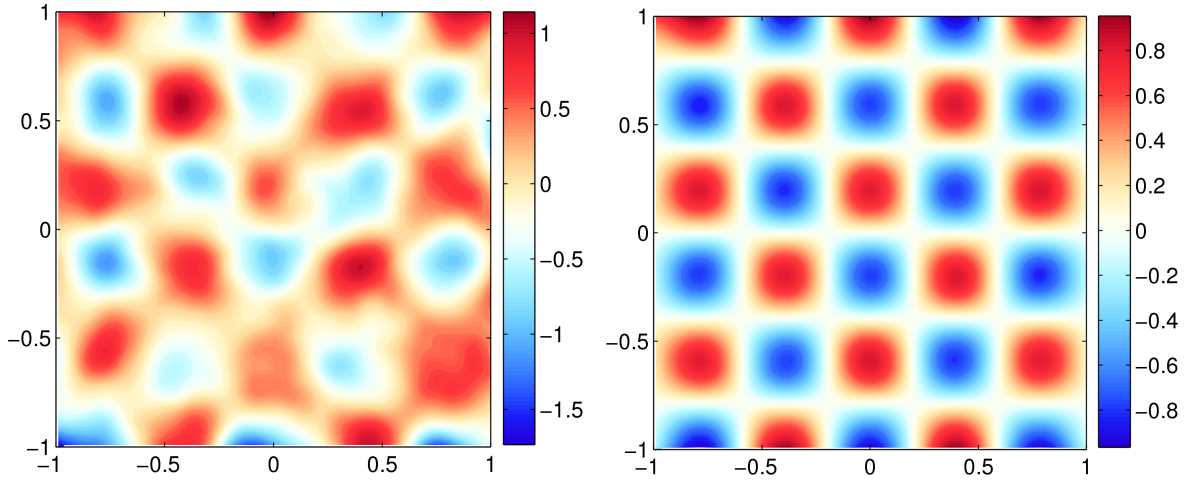


Figure 5.6: Example of a reconstruction without (a) and with detrending (b). Note the difference in the color bars.

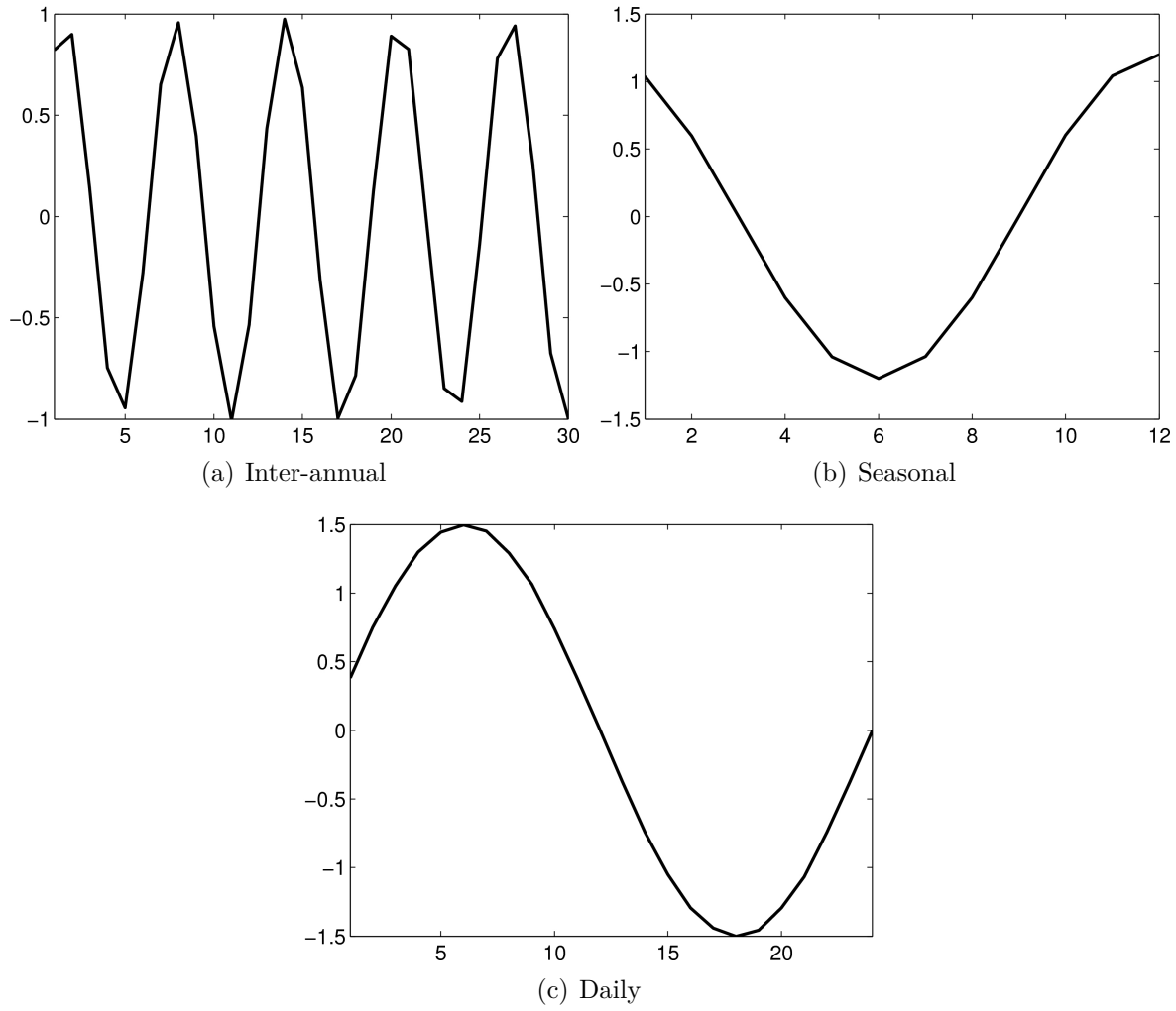


Figure 5.7: Trends obtained from the data using the detrending tool.

Part II

2-D implementation

6 Scripts, input files and directories

This chapter starts with the description of the scripts used by Diva, then input files required for simple 2-D analysis are presented here. Basically, only three files are needed as input:

1. a file containing the data (`data.dat`)
2. the specification of the domain of analysis (`coast.cont`) and
3. the list of the parameters used during the analysis (`param.par`).

Contents

Convention: Diva works with decimal numbers represented with . not ,

Tips 6.1 *Use unix command* `sed` *to replace* , *by* .*:*

```
[Software] cat file1.dat | sed s/,/./g > file2.dat
```

where: `file1.dat` *is the old file and*
`file2.dat` *is the file where the replacement has been made.* ■

Tips 6.2 *Use editor vi to replace* , *by* .*:*

Simply type:

```
[Software]$ vi file1.dat
:,$s/,/./g
```

■

6.1 List of 2-D tools

6.1.1 Operations on data

divabin: bins the data in order to improve the quality of the optimized parameters (CL and SNR).

divaanom: computes the difference between the data and the provided reference field.

divadataclean: eliminates all data that fall outside the bounding box of the contours.

divadatacoverage: Writes Relative Length (RL) (`RL.dat` and `RLInfo.dat`) field based on data coverage and data density field (`DATABINS.dat`).

dvncmask2RL: Writes Relative Length (RL) (`RL.dat` and `RLInfo.dat`) field based on a given mask on the domain.

6.1.2 Parameter estimation

divabestguess: provides estimates for the correlation length and the signal-to-noise ratio with methods chosen according to the number of data.

divacv: performs ordinary cross-validation.

divacvclasses: performs ordinary cross-validation by setting aside all data from a given class (e.g., specific year) and comparing the analysis to them.

divacvrand: performs cross-validation by taking out several points at once to calculate error estimates and repeat the exercise several times to make estimates robust.

divafit: estimates the correlation length by fitting the data correlation function to the theoretical kernel.

divagcv: estimates the signal-to-noise ratio by performing a generalised cross-validation.

divagcvalex:

divaguesssn:

divasnbygrid: creates a grid with noise level and data weights.

6.1.3 Contours and mesh

divacc: check the consistency of the initial contour file.

divacoa2cont: converting ODV-format coastlines to Diva-format coastlines.

divacont: creates the contours from a given bathymetry and a selected depth levels.

divacont2grid: translate contours into gridded format.

divamesh: generates the finite-element mesh.

6.1.4 Analysis

divabigtest: performs a test with a very large number of data points.

divacalc: performs the Diva analysis.

divadetrend: performs an analysis with the detrending option activated.

divadress: performs a complete analysis: cleaning (divaclean), mesh generation (divamesh), analysis (divacalc), outliers detection (divaqcbis) and outliers removal (dvoutlierclean)

divaintegral: compute the integral of the treated variable of the considered domain.

divamultivar: performs an analysis with the multivariate approach.

divarefe: computes a reference field with a semi-normed analysis with an increased value for L.

divaseminorm: performs an analysis with a semi-normed reference field: computes the reference field (divarefe), computes the anomalies with respect to the reference field (divaanom), makes the analysis (divacalc) and add the reference field to the obtained analysis (divasumup).

divasumup: performs the last step of a semi-normed analysis: the sum of background field and analysed anomaly field.

Analysis: using relative length field

divadatacoverage: Writes in `input` Relative Length (RL) field based on data coverage. RL fields are used to perform an analysis when they are present in `input`.

dvncmask2RL: Writes Relative Length (RL) field based on a given netcdf mask file of the domain. It uses the file `mask.nc` if present in `input` and writes `RL.dat` and `RLInfo.dat` to `input` directory.

6.1.5 Quality control and error field

divacpme: computes de the clever poor man's error.

divaexerr: advanced method to compute the exact error field.

divaqc, divaqcbis, divaqcter: performs quality control on data (see Section 3.3).

6.1.6 Misc

divaclean: cleans up the working directories by removing `fort.*` files from `divawork` and `meshgenwork`, as well as output files from `output`.

divagnu: prepares the plot of outputs using Gnuplot.

divaload: load the input files from a given directory.

divasave: saves the output files in a given directory.

6.2 Input files

6.2.1 Contour

The contour file (`coast.cont`) delimits the region where the analysis has to be performed, i.e., it specifies the boundary between land and sea. The file is defined this way:

1. The first line indicates the number of contours (M) in the region of interest.
2. The second line tells the number of points (N_1) in the first contour.
3. The next N_1 lines are the coordinates of the points of the first contour. The convention for the contour is that *the land is on the right when you follow the points successively*. The contour is automatically closed, meaning that the last point of a given contour is be from the first one.
4. The following line is the number of points (N_2) of the second contour.
5. ...

```
2
4
0 0
100 0
100 80
0 80
4
60 40
80 40
80 60
60 60
```

Example file 6.1: coast.cont

6. The last N_M lines are the coordinates of the points of the last contour.

Here, the contour is made up of 2 sub-contours:

- the first one with 4 points (and 4 edges): $(0, 0)$, $(100, 0)$, $(100, 80)$ and $(0, 80)$. It is the main contour.
- the second one with also 4 points. It is the interior contour (island).

In realistic application, the contours are more complex: they have more sub-contours (islands, interior seas), and each sub-contour is made up of more points.

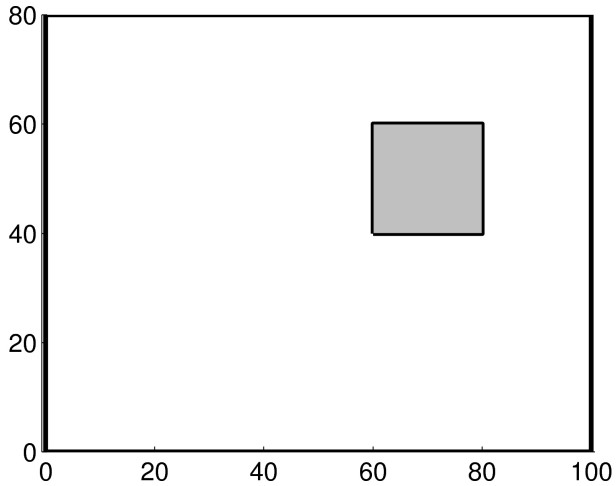


Figure 6.1: Example of a contour file and its graphical representation.

6.2.2 Data

The data file (`data.dat`) contains at least three columns:

1. the $x-$coordinate (usually the longitude, but can also be an horizontal distance in km, or any coordinate).

2. the $y-$coordinate (usually the latitude).
3. the data value.

- The fourth column [optional] indicates the weight of the each data point. If this column is empty, the fourth column is assumed to take the value 1.
- If there are more than four columns, columns 5 and higher are not used by the software, except if you want to use the detrending tool (Section 5.3).

```
20 10 3
60 20 -2
30 50 0
40 70 -1
70 70 -2
85 55 4
90 10 2
70 35 -4
```

Example file 6.2: data.dat

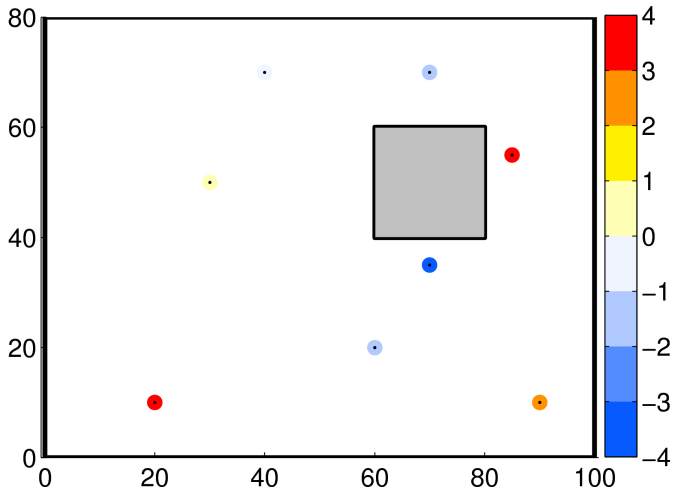


Figure 6.2: Example of a data file and its graphical representation.

6.2.3 Parameters

The file `./input/param.par` specifies the main analysis parameters and options of Diva. A clear understanding of is essential for a proper use of the software. A description of each parameter is provided below the example file.

Lc

The global correlation length L used for the analysis (see Section 2.3.1 for the physical meaning). It has to be defined as a real positive number. Note that the length of the finite-elements will be computed according to the value of L.

```
# Correlation Length lc
0.2
# icoordchange
0
# ispec
11
# ireg
0
# xori
0
# yori
0
# dx
0.02
# dy
0.02
# nx
51
#ny
51
# valex
-99
# snr
1.0
# varbak
1.0
```

Example file 6.3: param.par

As a first guess, you can use a value between a tenth of the domain size and the domain size, in order to avoid getting into memory troubles due to a too fine mesh. Later, you can change this value if it seems interesting (via optimization).

`icoordchange`

Specifies the desired type of coordinate system:

`icoordchange` = 0 if no change is necessary (same coordinates as data);
= 1 if data positions are given in degrees and if you want to use real distances;
= 2 if data positions are given in degrees, you want to use real distances, and your domain extends on a wide span of latitude (uses a cosine projection);
= $-xscale$ to scale x coordinates by a factor $xscale$ before doing anything (for vertical sections: see Section 10.2)

`ispec`

Four base-values specify the required error outputs:

`ispec` = 0 : no error field requested
= 1 : gridded error field specified by `xori`, `yori`, `nx` and `ny`;
= 2 : errors at data locations;
= 4 : errors at locations listed in `valatxy.coord`.

Then you can combine these four values to obtain several error outputs:

Examples

`ispec` = 3 (=1+2) means you want gridded error field as well as errors at data locations;
`ispec` = 7 (=1+2+4) means you want the three error files.

From there several variants can be specified:

For computing errors with the real covariance function (Section 4.1.4), simply multiply the `ispec` value by −1:

Example

`ispec` = -7 means you want the three error files computed with the help of the real covariance function.

For computing errors with the real covariance function using boundary effects (Section 4.1.4), simply add −10 to a negative `ispec`:

Example

`ispec` = -17 means you want the three error files computed with the help of the real covariance function and boundary effects.

A *poor man's* error estimate (quick and underestimated error field, Section 4.1.1) is available by adding +10 to the positive base `ispec` value:

Example

`ispec` = 16 means you want errors at data locations and at points listed in `valatxy.coord` computed with the *poor man's* error estimate.

Adding +100 to the base `ispec` activates the clever poor man's error calculation and launches automatically `divacpme`

Example

`ispec` = 116 means you want errors at data locations and at points listed in `valatxy.coord` computed with the *clever poor man's* error estimate.

Adding −100 to a negative `ispec` activates the almost exact error calculation and launches automatically `divaexerr`

Example

`ispec` = -106 means you want errors at data locations and at points listed in `valatxy.coord` computed with the almost exact error estimate.

Example

`ispec` = -117 means you want errors everywhere computed with the almost exact error estimate using the background covariance with boundary effects.

`ireg`

Specification of the background field which is subtracted from the data field (Section 2.3.1).

`ireg` = 0 : no background field is subtracted (assuming data are already anomalies);
= 1 : the data mean value is subtracted;
= 2 : the linear regression of the data (plane) is subtracted.

`xori/yori, nx/ny`

`xori/yori` indicate the coordinates of the first grid point while `nx/ny` indicate the number of grid points in `x/y` directions.

`valex`

Exclusion value: value used to fill the output matrix when a point corresponds with land. Any value is accepted, but the user has to ensure that the exclusion value cannot be a value obtained by the interpolation of the measurements.

`snr`

Signal-to-noise ratio of the whole dataset (Section 2.3.1). It has to be defined as a real positive number (as the correlation length).

varbak

Variance of the background field.

6.2.4 Locations of additional points where analysis is required (optional)

The file `valatxy.coord` is a two-column list of locations where you want the analysis to be performed (in addition to the regular grid defined in `param.par`).

```
20 20 0
60 10
40 40
```

Example file 6.4: valatxy.coord

If they exist, columns 3 and higher are not used.

6.3 Working directories (2-D analysis)

For 2-D analysis, the main working directory is `divastripped`. Inside it, we have:

```
[divastripped] tree -d -L 2
.
|-- divawork
|   `-- sub
|-- gnuwork
|   |-- gnuplottools
|   `-- plots
|-- input
|-- meshgenwork
`-- output
    |-- ghertonetcdf
    `-- meshvisu

10 directories
```

divawork is where the intermediate files are produced.

gnuwork contains the scripts for generating the plots with Gnuplot. These plots will be located in the sub-folder `plots`.

input contains the input files presented in this section.

divawork is the working directory for the mesh generation.

output contains the analysis results. In `ghertonetcdf`, one can find the output in NetCDF format (file `results.nc`), while `meshvisu` stores the files that describe the mesh.

7 Preparation of the input files

We describe in this chapter the tools to prepare the various input files presented in Chapter 6. If you already have the input files at your disposal, you way want to go directly to the next chapter.

Contents

7.1 Creation of topography

A topography may be the first thing you have to prepare in order to generate a climatology. They are necessary in two cases:

1. when you need contour files at different depths to perform analysis;
2. when you work in a vertical plane and want to interpolate several profiles from a cruise.

Basically, the procedure consists in creating files with a format readable by Diva. The list of methods presented in this Section is not exhaustive, but corresponds to different procedures to create topography files using different data bases freely available on the web.

> **Convention:** Diva works with the convention that depth are positive under the sea level. This is especially important when creating contours. Matlab tools provided with the software create topographies which respect this convention, but in case that you work with topography database that are not described in the following section,

Tips 7.1 *A simple way to change the sign of a given column of a data file is to use the following command:*

```
awk '{print $1,$2,-$3}' infile > outfile
```

where ***infile*** *is the old file and* ***outfile*** *the new one.*

If you need to switch two columns of a file, type:

```
awk '{print $2,$1,$3}' infile > outfile
```

■

7.1.1 Method 1: using Diva on web

Go to http://gher-diva.phys.ulg.ac.be/web-vis/diva.html, upload any data (it can be the example provided on the web). It is faster to use a small file, and you can even create a simple file with 2 measurements in the lower left and upper right corners of your region.

```
lonmin latmin value
lonmax latmax value
```

Then specify the output grid on the region where you want the topography and provide the resolution which is typical for the resolution you will use later for the analysis. Perform the analysis with your "data". In the download section, you can download the topography in a NetCDF file `diva_bath.nc`. Save this file into your `input`. Then on the command line, placed in this `input`, execute `../../bin/divabath2topogrd.a`. This will create `topo.grd` and `TopoInfo.dat`.

If you need to erase some zones from your topography, you have to create a netcdf file `masktopo.nc` before executing `../../bin/divabath2topogrd.a`. This `masktopo.nc` has

to be a 2D file containing a binary variable called MASKTOPO (0 where you want to erase the topography, 1 elsewhere). The dimensions have to be the same as `diva_bath.nc` and the axis have to be named "lon" and "lat" or "LON" and "LAT".

7.1.2 Method 2: conversion from GEBCO topography

The GEBCO bathymetry is distributed by the British Oceanographic Data Centre (BODC). If you have already registered, you can log in (https://www.bodc.ac.uk/my_account/login/), otherwise it is necessary to register to become a new user.

Download the complete, global GEBCO One-Minute Grid file (`90n90s180w180e.zip`) from http://www.bodc.ac.uk/data/online_delivery/gebco/ and unzip it to obtain the file `GridOne.grd`. Download the software `GebcoCE_GridOnly` as well and run it (on Linux : open the .exe with Wine).

Select your area

Select your region of interest (Fig. 7.1), possibly slightly increased to make sure boundaries are well included in the topography. Then select `File->Export Data->Gridded Data`. Chose Ascii longitude-latitude-depth (default). For the longitude range, use `-180:180` for European seas. Note regions you possibly want to mask later by their coordinate ranges. Use `topo.gebco.asc` as output file name, into a directory where you have your main climatological working place. Push `OK` and be patient. (Fig. 7.2).

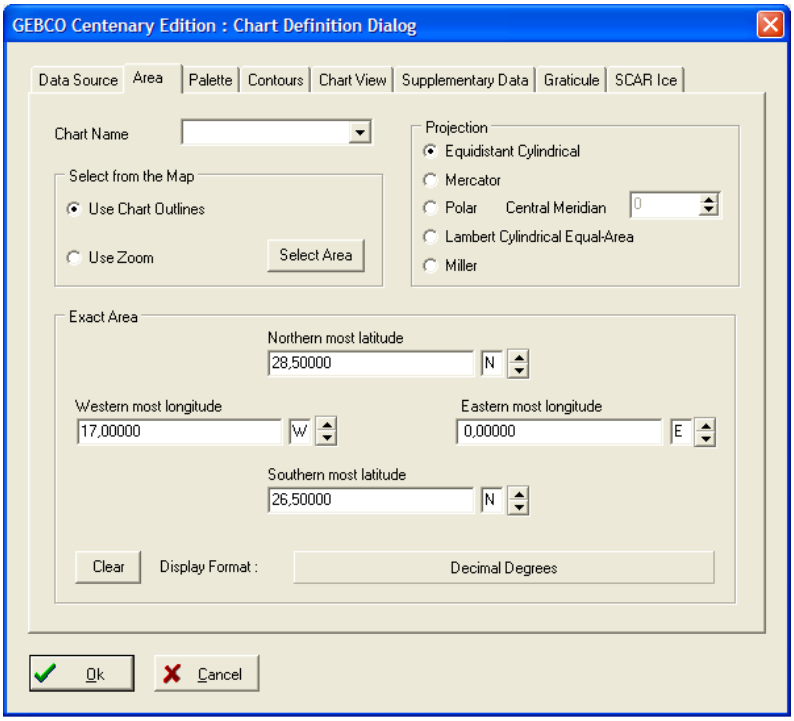


Figure 7.1: Area selection with software `GebcoCE_GridOnly`.

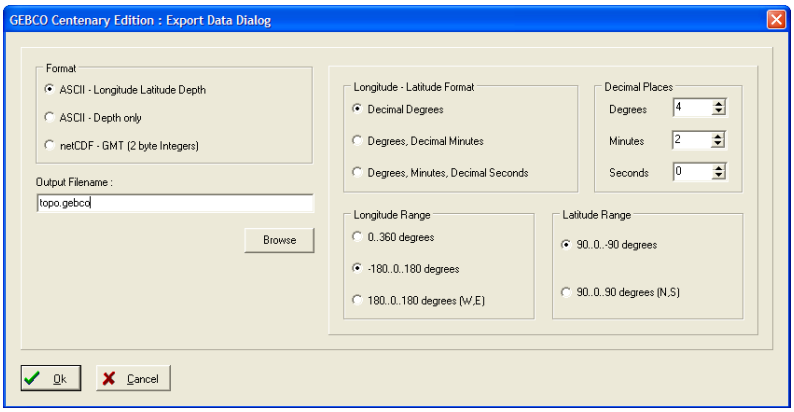


Figure 7.2: Data exportation with software ***GebcoCE_GridOnly****.*

Convert the file into gher format

Go into Cygwin (or into Linux mode) and place yourself in the main directory of your climatology production. You should have a big `topogebco.asc` file on which you can apply

```
[ input] head -20 topogebco.asc
```

to see if the file was created correctly. You also should have a `gebcoprep` file. If not, copy the `gebcoprep.example` file as `gebcoprep`.

If you need to mask regions, edit `gebcoprep` and add lines as those put with `#awk` followed by `#mv bidon`. They should be self explaining and allow excluding regions that are defined by relationships between longitude and latitude.

Example `(2 > 57.0 + 0.6*1) x=-10.` means that regions where latitude is larger than `57+0.6*longitude` will be masked.

Once you defined the regions to be masked in this way, execute `gebcoprep`. When working on large domains, the computation time can be very long. However, this step has not to be repeated a lot of times. The execution of `gebcoprep` will create an ascii file called `./input/topo.gebco`.

Now you are ready to prepare the gridded topography `topo.grd` from which Diva will extract contours. To prepare it, copy or move `./input/topo.gebco` into the diva working directory to have `divastripped/input/topo.gebco`.

The best resolution offered by GEBCO is 30-arc seconds, which might be much too fine for large scale analysis. To avoid that, run `gebco2diva` with optional arguments `nx ny` to make a grid using only every `nx` point in $x-$direction and `ny` in $y-$direction. For example, if you are interested in a Diva output resolution that is working at a 100 km scale, `gebco2diva15 15` would still provide a very fine topography with respect to the scales of interest.

In the `divastripped` directory, the execution if `gebco2diva` will generate two files in `divastripped/output/` for describing the topography:

`topo.grd`: a binary file containing the gridded topography.

TopoInfo.dat: a ascii file describing the topology of the grid and similar to GridInfo.dat.

You can further check the two files by copying them into the divastripped/input directory and executing divacont and divagnu. If results seem right, you can save the files TopoInfo.data and topo.grd into your main data directory, to be used with divacont on all levels defined by contour.depth.

If everything is stable, you can erase topogebco.asc and topo.gebco to save disk space.

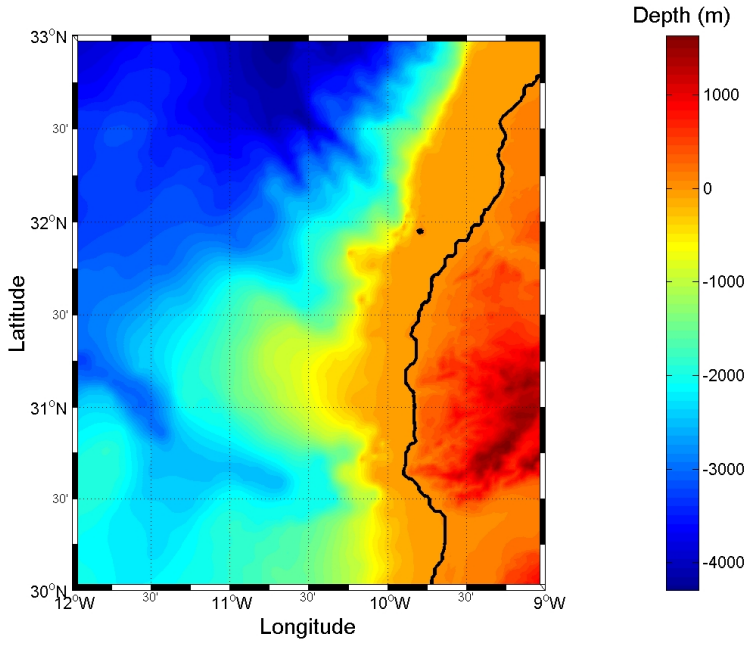


Figure 7.3: Topography from GEBCO one-minute topography.

7.1.3 Method 3: interpolation of individual topography measurements

The principle of this method is to apply a Diva analysis to a data file containing depths at various locations.

Get topography measurements

In the present example data points are extracted from http://topex.ucsd.edu/cgi-bin/get_data.cgi in the same region as the previous case ($9-12°W \times 30-33°N$). The output file is composed of three column: `| longitude | latitude | depth |`, i.e., the same format as data.dat files used by Diva. Once the file is downloaded, edit its name in topo.dat. Figure 7.4 shows the individual measurements (coloured dots) in the region of interest.

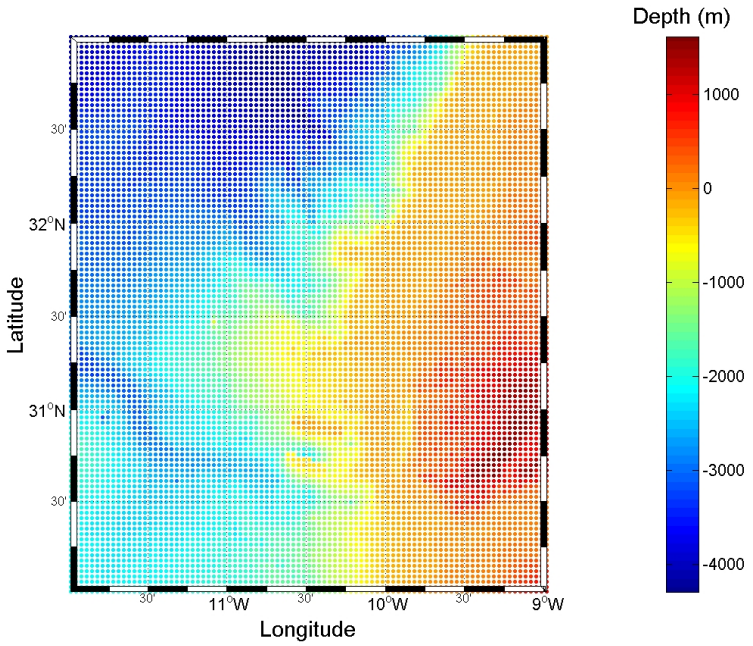


Figure 7.4: Individual measurements of depths.

Adapt parameters

As in any Diva analysis, you need to provide parameters concerning the analysis itself and the output grid (file `param.par`, described extensively in Section 6.2.3, page 62).

- Correlation length is chosen according to the resolution of the gridded topography you extracted, i.e., the distance between two measurements.
- Signal-to-noise ratio is assigned with a large value (typically 100 or more).
- `x/yorigin` are chosen according to the region where you extracted data.
- `dx` and `dy` are the same as the values you use for your analysis.

Execute `divatopo`

With the two files `topo.dat` and `param.par` located in `divastripped/input/`, type `divatopo` to launch the analysis. `divatopo` automatically creates a contour file according to grid parameters taken in `param.par`. The interpolated field is presented on Fig. 7.5. Outputs `topo.grd` and `TopoInfo.dat` may then be used to generate contours (see Section 7.2).

7.1.4 Method 4: by hand

Create a gridded file (in the same format as the analysis fields `fieldgher.anl`) of topography and call it `topo.grd`. The information on the grid's geographical dimensions are to be placed in `TopoInfo.dat`.

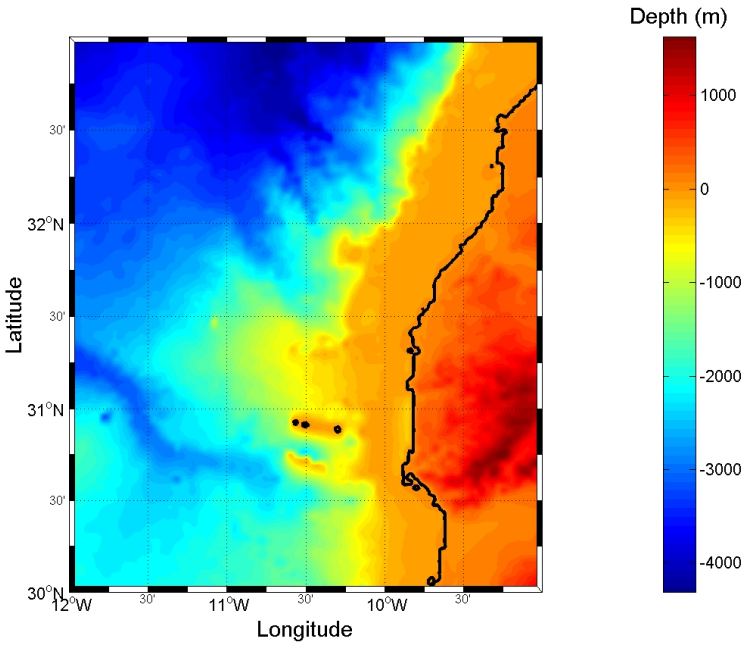


Figure 7.5: Interpolated topography.

The grid is simply an array $(i = 1, \ldots, M)$ and $(j = 1, \ldots, N)$, where the coordinates of the grid nodes are $x_i = x_1 + (i-1) * dx$, $y_j = y_1 + (j-1) * dy$. The file `TopoInfo.dat` contains simply

```
x1
y1
dx
dy
M
N
```

Look into `dvdv2diva.f` in `./src/Fortran/Util/` how to write such files from within a Fortran code.

7.1.5 Deprecated method: conversion of data from Topography Extractor

This DBDB-B topography is not available any more, hence the method described below cannot be used. It is kept in this manual for compatibility purposes.

Select your area

Go to https://idbms.navo.navy.mil/dbdbv/dbvquery.html, select the area and spacing and download the corresponding file in `CHRTR ascii` format (Fig. 7.6). In this example we worked in the region delimited by $[9-12°W \times 30-33°N]$ (NW Africa) with a resolution of $0.01°$ in both directions.

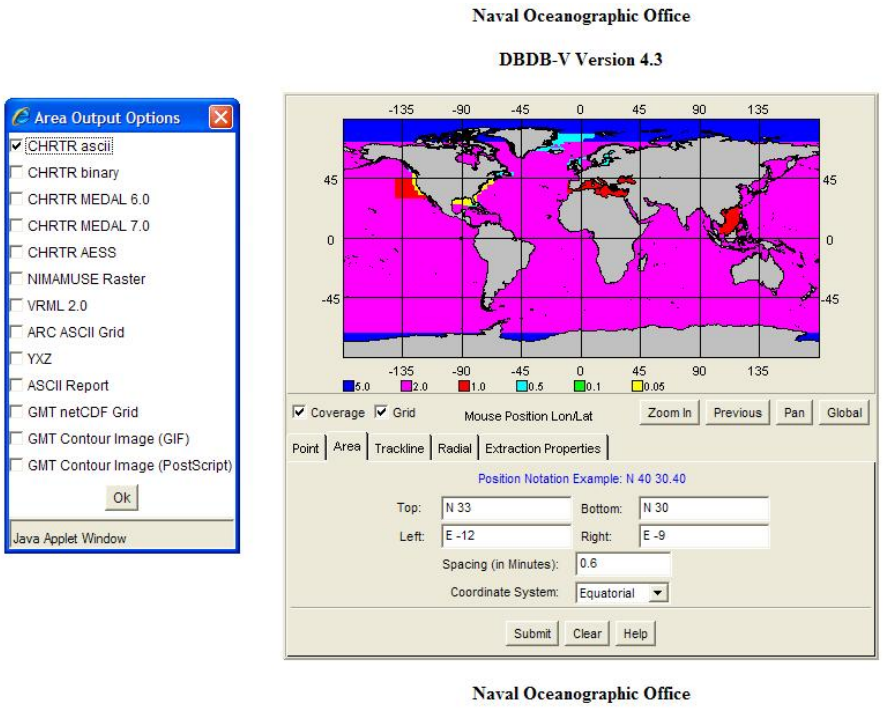


Figure 7.6: Topography extraction from the Naval Oceanographic Office website.

If the web server is not operational, you can also access this database at http://ferret.pmel.noaa.gov/NVODS/servlets/ Then select your dataset by clicking on "*by Dataset Name*" and chose "*NAVAL OCEANOGRAPHIC OFFICE Bathymetry/Topography 5min resolution*".

Mark the topography box and click on "*Next*" (Fig. 7.7(a)).
Delimit your region and select "ASCII file" as output (Fig. 7.7(b)).

Put the `.asc` file into `divastripped/input/` with the name `topo.asc` and execute `dbdb2diva` in the shell. You will get `topo.grd` and `TopoInfo.dat` in the `output` directory. The corresponding topography is drawn on Fig. 7.8.

7.2 Creation of contours

As seen in first chapter, a relevant asset of Diva is the fact that it takes into account real coastlines and topography of the region of interest. We explain hereinafter the techniques to produce a correct coastline file, of which the description is provided in Section 6.2.1.

7.2.1 By hand

The first possibility is to build your file *by hand*: having at your disposal the location of different points of the coast (longitude, latitude), simply create a file containing M contours, with the $i-th$ contour having being made up of N_i points ($i = 1, 2, \ldots, N$).

Be aware that some cases (Fig. 7.9) are to be avoided, since problems arise during the mesh generation when crossings occur in the contour. Also note that, as contours are automatically closed by Diva, the segment joining the first and the last points may generate

(a)

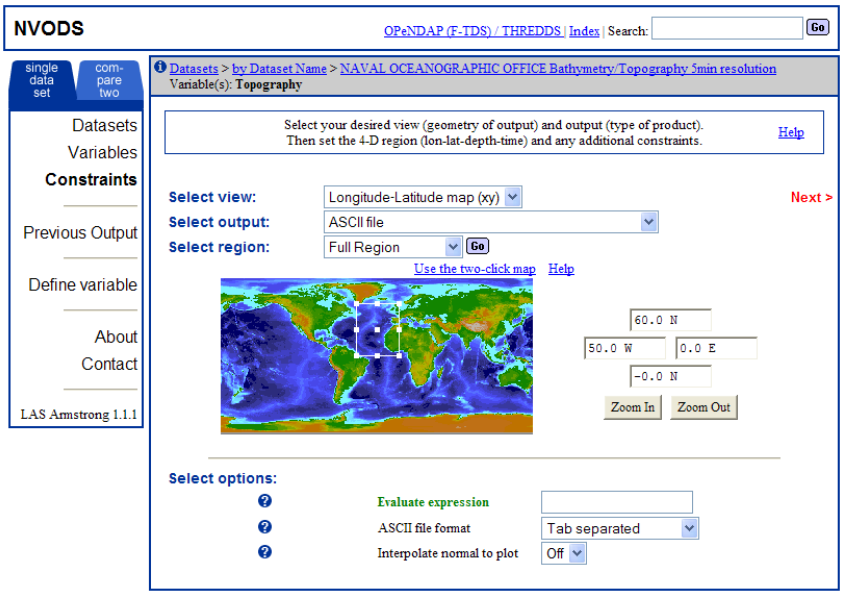


Figure 7.7: Topography extraction from NVODS.

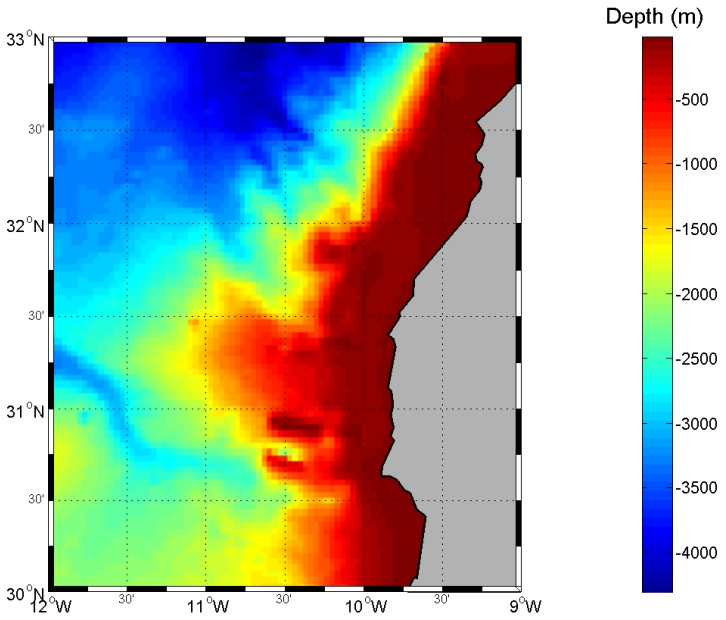


Figure 7.8: Topography from Naval Oceanographic Office website.

errors.

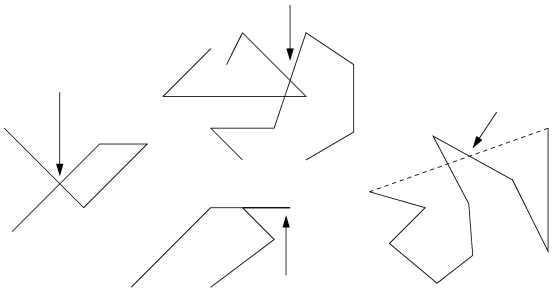


Figure 7.9: Example of improper contours. Left: crossing of two segments of a same contour; up: crossing of two different contours; right: first and last points of the contour generate a segment that crosses the other parts; down: two contours having a common segment.

Remember that you can use the tool `divacck` for checking and thinning of contours.

7.2.2 From topography

Once you have placed files `topo.grd` and `TopoInfo.dat` in directory `./input`, type `divacont` in the command line shell. This will generate several coastline files named `coast.cont.100nn`, where *nn* corresponds to the nn^{th} level defined in `contour.depth`. File `coast.cont` contains the coastline at the surface level ($z = 0$).

As an illustration, we want to have contours from surface to a depth of 1000 m every 200 m, with `topo.grd` and `TopoInfo.dat` created in the Section 7.1. To this end we use the following file:

Contours for the specified depths are showed on Fig. 7.10.

```
2500
2000
1500
1000
500
0
```

Example file 7.1: contour.depth

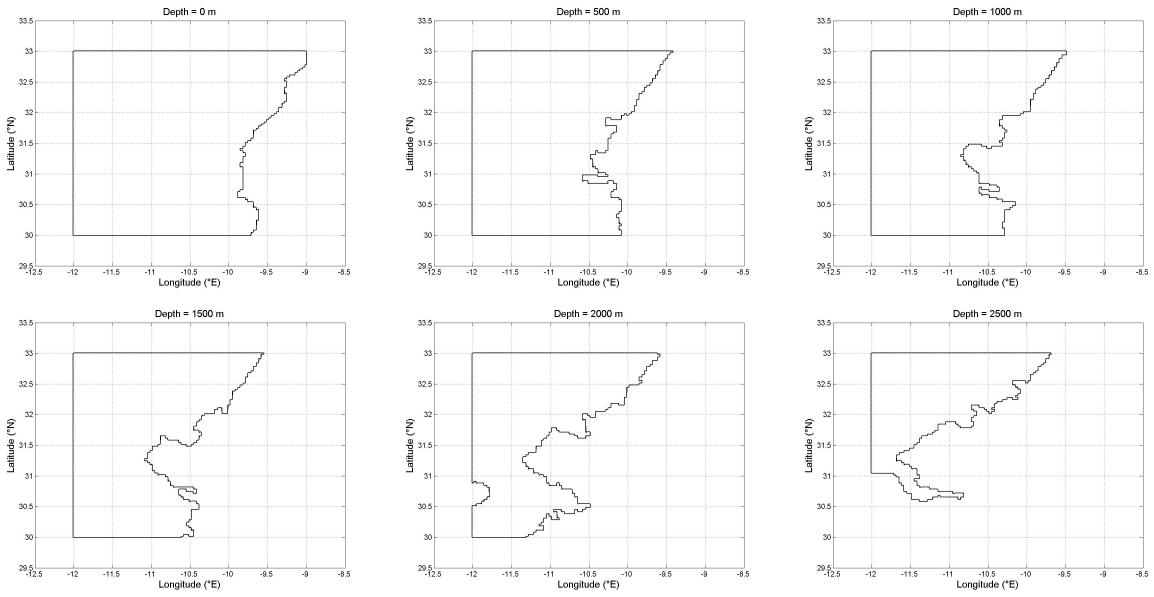


Figure 7.10: Contour generated every 500 m from surface to -2500 m.

7.2.3 Using ODV

Tool `divacoa2cont` allows converting ODV-format coastlines to Diva-format coastlines. Simply copy coastline file in the `input` directory with the name `coast.coa` along with a `param.par` file and type `divacoa2cont` in the shell.

This provides you the new file `./input/coast.cont`.

7.2.4 From a mask

Simply look at `contourgen.f` and create the mask as you wish. Alternatively you can create a pseudo-topography with adequate pseudo-depth at which you draw the contour.

7.3 Determination of analysis parameters

Two key parameters have to be adjusted before running an analysis: the correlation length scale (L) and the signal-to-noise ratio (λ). Several tools are provided in order to help the user for the determination of these parameters.

7.3.1 `divafit`

The script `divafit`: uses the data (`./input/data.dat`) for a direct fitting of the covariance function (see Section 2.3.3). Note that the fit needs a sufficiently large data set.

Command description

`divafit` : performs a fit of the data correlation function based on the whole data set.
`divafit -r` : puts the new value of L in `param.par` in function of the fit.
`divafit n` : performs the fit on a sample of `n*(n-1)/2` couples of data (sub-sampling).

Example
`divafit -r 100`: performs a fit on 4950 couples of data and update the file `param.par`.

Tips 7.2 *When dealing with very large datasets, using `divafit` with sub-sampling may save you a large amount of time.* ■

Note when using advection constraint and variable L, `divafit` will not provide a very meaningful value.

Output files

In output file `./output/paramfit.dat`, the best estimates are given and could be used as parameter values for running Diva. Estimates of the correlation length are rather robust while those of the signal-to-noise ratio are neither precise nor robust, especially for large values.

Output file `covariance.dat` is the data-based covariance function:

column 1: distance between points,

column 2: covariances,

column 3: number of data couples used to estimate the covariance.

Output file `covariancefit.dat` allows looking at the fitted covariance function:

column 1: distance between points,

column 2: data-covariance,

column 3: fitted covariance.

Finally, file `param.par.fit` is the original `param.par` file except that the correlation length has been replaced by the fitted value.

Note always have a look at the fit to judge on its quality.

7.3.2 divagcv

The script `divagcv` exploits Diva module (`gcvfac`), analysing random fields to assess the generalized cross validator (GCV, see Chapter 3 for theoretical developments). The script `divagcv` is an example of how to minimize the estimator by changing the signal-to-noise ratio (λ) value, but could be adapted to optimize other parameters as well, such as correlation length.

Input to the module is the number of random estimates required (the larger the value, the more robust the estimator). Default value is 5, unless you change in `divacalc`. The user has to provide an input file `./input/gvcsampling.dat` containing the list of values for λ on which to try the estimator (typically around the values provided by `divafit`).

During the `divagcv` execution, error-field calculations are disabled to reduce computing time.

Tips 7.3 *If a mesh already exists (in `meshgenwork` directory), `divagcv` disables the `divamesh` procedure. For this reason, ensure you are working with the adequate mesh.* ■

Output files

File `./output/gcv.dat` contains the GCV estimator:

column 1: signal-to-noise ratio,

column 2: GCV,

column 3: data anomaly variance.

and `./output/gcvsnvar.dat` the best new estimate for the S/N and `VARBAK` parameters.

In `param.par.gcv`, you find an adapted version of the original `param.par`.

7.3.3 divabin

`divabin` performs a spatial binning of the data with the spatial resolution defined in `param.par`. The script is called by `DIVA3D/divastripped/divafit` (for CL) and/or by `DIVA3D/divastripped/diva3Dsnop` (for SNR, only called when working in 3 or 4D) if the parameter "binning" is set to the value "1" in these scripts (at the beginning). The purpose of this optional binning is to improve the quality of the parameters (CL and/or SNR) optimization by averaging a part of the highly correlated observations (taken by a boat in a restricted area, for instance).

7.3.4 divacv

`divacv` carries out a cross validation, point by point, without new matrix inversions.

7.3.5 divacvrand

`divacv` runs a cross validation by sub-samples of points.

Note in the present version (Diva-4.7.1), tools `divacv` and `divacvrand` do not adapt the error norm to include the relative weights on data. This will be introduced in the next versions.

7.4 Format conversion tools

7.4.1 ncdf2gher

`ncdf2gher` performs a format conversion from a 2D NETCDF file to a file in GHER format, with its info file (ASCII). The netcdf file `myfield.nc` has to be placed in `input`. Its axis have to be "lon" and "lat" or "LON" and "LAT". Only one variable (myfield, i.e. the name of your field) is accepted.

To launch the conversion, just type

```
[DIVA3D/divastripped] ./ncdf2gher myfield
```

Your variable "myfield" will then be stored into a gher format file named `myfield.grd` and its info file `myfieldInfo.dat`. These two files are in `input` and have the same form and conventions as `topo.grd` and `TopoInfo.dat`. By default, the exclusion value will be 10^6.

7.4.2 gher2ncdf

`gher2ncdf` performs a format conversion from a file in GHER format, with its info file (ASCII) to a 2D NETCDF file. The gher file `myfield.grd` has to be placed in `input`, as well as its info file `myfieldInfo.dat`. These two files have the same form and conventions as `topo.grd` and `TopoInfo.dat`.

To launch the conversion, just type

```
[DIVA3D/divastripped] ./gher2ncdf myfield
```

Your variable "myfield" will then be stored into a netcdf file named `myfield.nc`. Its axis will be "lon" and "lat". The exclusion value will be the same as in gher file. Only one variable (myfield, i.e. the name of your field) is accepted.

7.5 Misc

7.5.1 divaclean

`divaclean` cleans up the working directories by removing `fort.*` files from `divawork` and `meshgenwork`, as well as output files from `output`.

7.5.2 divadataclean

Script `divadataclean` takes the input data `./input/data.dat` and eliminates all data that fall outside the bounding box of the contours (i.e., the rectangle containing the analysis mesh). This avoids loading unnecessary large input files. If two additional arguments n_1 n_2 are added, data values falling outside the range specified by n_1, n_2 are also eliminated.

Example

```
[divastripped] divadataclean -3 35
```

will remove all data points of which the value is not between -3 and 35.

The output overwrites `./input/data.dat` but keeps the original one in `./input/` with the name `data.dat.full`. The tool should be used just after having loaded the data set (typically after `divaload`).

7.5.3 divaload

divaload loads input files from the chosen directory into divastripped/input/. You just have to specify the directory where your input files are located (relative or absolute paths). It is assumed that the input files are located in a folder input within the chosen directory.

Example

```
[divastripped] divaload ~/DIVA/test/
```

will load the files from ~/DIVA/test/input.

Tips 7.4 *When you want to know to which correspond the data present in the input directory, simply read the content of the file input/casename; it indicates the repertory from which you loaded input files with command divaload.* ■

7.5.4 divacck

divacck checks your initial contour file ./output/coast.cont. In output ./output/-coast.cont.checked you will find a thinned contour based on the length scale, where the possible couples of identical points are eliminated.

Application of divacck is normally not necessary if you created the contours with divacont.

8 Running analysis

Once all the input files are prepared, you are ready to create analysed gridded fields. The whole procedure is described in the present chapter.

Contents

8.1 Running a simple analysis

8.1.1 divadress

The simplest procedure to carry out an analysis with Diva is using the command divadress, which performs the four following operations:

1. divaclean
2. divamesh
3. divacalc
4. divaqcbis

8.1.2 divamesh

Generates the finite-element mesh based on contour(s) specified in file `coast.cont` and correlation length provided in `param.par`; remember that the correlation length shall have an appropriate value in order to obtain a correct mesh:

- Contour segments should not be much smaller than finite element length; if your contour is too fine, the tool `divacck` can be used in order to reduce the contour resolution.
- The typical length of a finite element should be smaller than the correlation length, otherwise the grid would be too coarse compared to the signal to resolve.

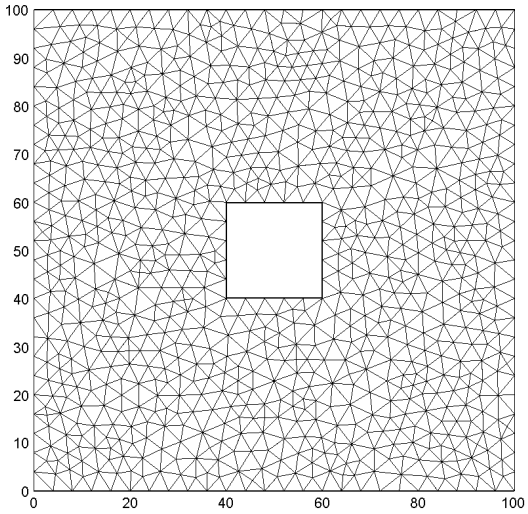


Figure 8.1: Mesh on a simple domain.

Note since version 4.3, mesh generation takes into account coordinate change (specified by `icoord`) so that meshes are uniform in the transformed domain.

Mesh with different element sizes

You also have the possibility to create of mesh of which the size of the elements varies over the domain. To this aim, you have to create a *mesh density* file that indicates what length scale has to be applied in a determined region. This file is named `coast.cont.dens` and has to be placed in `divastripped/input/`.

We considered the simple island case, of which the contour file given by

We choose a value of 2.5 for the global mesh (specified in `param.par`) and define a finer mesh around the island through the following `coast.cont.dens` file:

which means that we want a length scale of 0.125 in the domain defined by by the four points (1 1), (4 1), (4 4), (1 4). Be sure that the domain where you want to have a finer mesh is on the left when following the contour. The mesh generated with these conditions is presented on Fig. 8.2.

```
2
4
0 0
5 0
5 5
0 5
4
2 2
2 3
3 3
3 2
```

Example file 8.1: coast.cont

```
1
0.125 4
1 1
4 1
4 4
1 4
```

Example file 8.2: coast.cont.dens

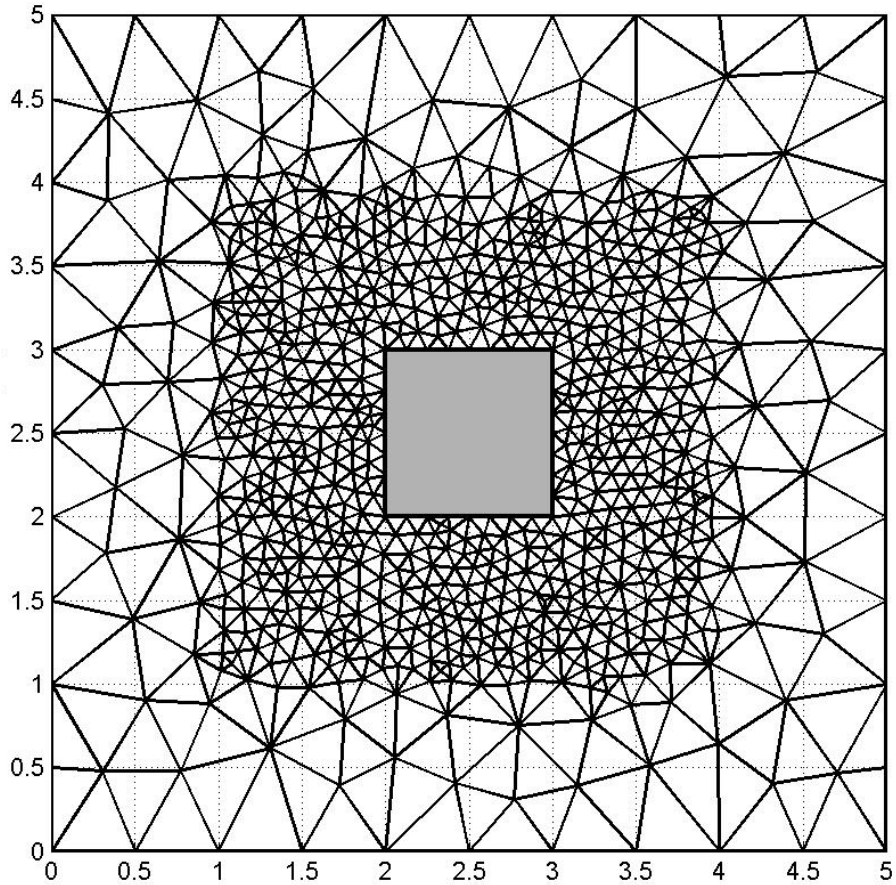


Figure 8.2: Mesh refinement around the island.

8.1.3 divacalc

divacalc is the script that runs the analysis by solving the variational principle over the domain of interest. To work properly, it needs a data file, a parameter file, and a finite-element mesh.

Tips 8.1 *As the mesh generation is often the most time-consuming part of a* Diva *execution, remember that once you have created the mesh, you do need to run* divadress *each time you want a new analysis, but just* divacalc. ■

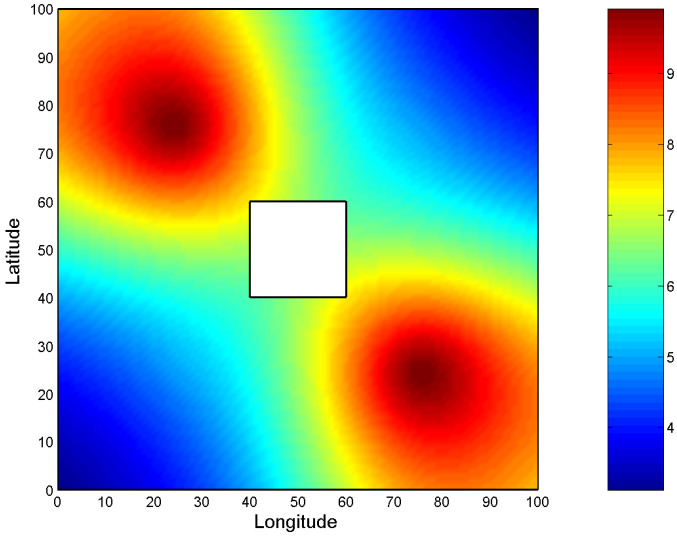


Figure 8.3: Example of analysed field.

Output files

- fieldgher.anl and errorfieldgher.anl are respectively the analysis and the error fields (in gher format) on the regular grid specified in param.par;
- fieldascii.anl and errorfieldascii.anl are the same as fieldgher.anl and errorfieldgher.anl, but in ascii format;
- valatxyascii.anl and erroratxyascii.anl give respectively the values of the analysis and the error fields at the points specified in file valatxy.coord;
- fieldatdatapoint.anl and erroratdatapoint.anl are respectively the analysis and error fields computed at the data points (*i.e.* the points from data.dat);
- results.nc (located in ./output/ghertonetcdf) is a NetCDF file containing the gridded analysis and error fields (provided error calculation is switched on).

8.2 Quality control of data

According to theoretical developments of Chapter 3, quality control with Diva can be performed using to one of the three criteria (3.24), (3.25) or (3.26), respectively implemented

in Diva with `divaqc`, `divaqcbis` and `divaqcter`.

8.2.1 Tools

There are three tools to perform QC:

`divaqc`: it is the most expensive version of QC, since A_{ii} must be evaluated by analysis of vectors with zeros everywhere, except at the i^{th} position.

`divaqcbis`: this version of the QC is quicker, as we replace A_{ii} by its average $\frac{1}{N}\text{trace}\,(\mathbf{A})$.

`divaqcter`: the last criterion implemented is based on the RMS value of the misfit and the generalized cross validator Θ.

8.2.2 Output files

The corresponding outputs are given in `outliers.dat`, `outliersbis.dat` and `outlierster.dat`. The modules `divaqc*` also generate `outliers*.normalized.dat`, which contain, in a sorted way (from the most suspect data to less suspect), the possible outliers from the normalized misfits test (3.29).

Tips 8.2 *By default, the criterion used in `divadress` is `divaqcbis`, but you can change it by editing the file `divadress` and replacing `divaqcbis` by one of the other quality test (`divaqc` or `divaqcter`).* ■

8.3 Running a semi-normed analysis

A semi-normed analysis consists of four steps:

1. create a so-called *reference field*, which will act as background field (Section 2.1.2);
2. subtract the reference field from the data values in order to work with anomalies;
3. perform an analysis on the anomalies;
4. reconstruct the field by adding the analysed anomaly field to the background (reference) field.

These four steps are executed by running script `divaseminorm` and the implemented tools described hereinafter. Note that the parameters written in the original `param.par` file will be used during the analysis on the anomalies. Thus it is advised to specify `ireg`=0, so that no background field will be subtracted from the anomaly.

8.3.1 `divarefe`

This script performs an analysis on your original data, but modify the analysis parameters: L is multiplied by 5 and λ by 0.1.

Output files

They are the same as those created through an execution of `divacalc`, but assigned with a suffix `.ref`: `fieldgher.anl.ref`, `fieldascii.anl.ref`, `valatxyascii.anl.ref` and `fieldatdatapoint.anl.ref`.

8.3.2 `divaanom`

The script use file `fieldatdatapoint.anl.ref` to compute the difference between data and analysed (reference) field to obtain anomalies.

Output files

File `data.dat` contains anomalies instead of the original data, while file `data.dat.full` is the copy of your original data file.

8.3.3 `divacalc`

This command was previously described (Section 8.1.3). The only difference is that it is applied here on anomalies.

8.3.4 `divasumup`

`divasumup` performs the last step of a semi-normed analysis: the sum of background field and analysed anomaly field.

Output files

They are the same as those created through an execution of `divacalc`. Note that after an execution of `divasumup`, `data.dat` contains the original data, while `data.dat.anom` contains the previously computed anomalies.

8.4 Extras

8.4.1 Saving outputs

`divasave` is designed for saving the outputs in the folder `output` to the chosen directory.

Example

```
[divastripped] divasave ~/DIVA/test/
```

will save the files into `~/DIVA/test/`

8.4.2 Checking of installation

`divacheck` makes the comparison of analysis results with reference analysis (for installation check, compiler option testing or checking of new versions)

8.5 Analysis with advection constraint activated

The input files needed for such analysis are the same as for a basic analysis, except that you need to provide a velocity (or pseudo-velocity) field, specified through the following files:

- `Uvel.dat` and `Vvel.dat`, which contain the two components of the velocity. They have the same format (binary) as `fieldgher.anl`. An example of generation of such files is in the test case `advectiontest`.
- `UVinfo.dat`, which specifies the grid on which the velocity field is defined. It has the same format as `GridInfo.dat` or `TopoInfo.dat`).
- `constraint.dat`, which activates the advection constraint and contains parameters θ and $\mathcal{A}$. Refer to Chapter 5 for theoretical details.

```
 -3.
-3.
0.100000001
0.100000001
61
61
```

Example file 8.3: UVinfo.dat

```
 100 0.0
```

Example file 8.4: constraint.dat

8.5.1 Interplay with coordinate change on

In this example, we work on a region $[-1, 1] \times [59, 61]$ with $L = 0.2$ and $\lambda = 1$.

With no coordinate change (i.e., `icoordchange=0` in `param.par`), coordinates are taken as such and a single point in the center leads to an analysis that is circular when axes on x and y are drawn with equal scales (Fig. 8.4).

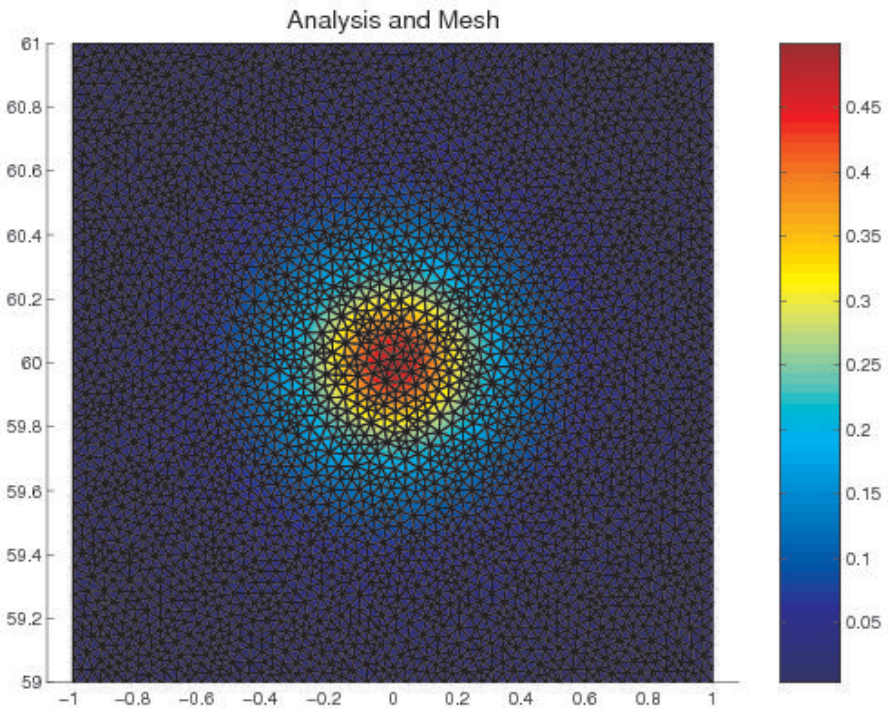


Figure 8.4: Analysis without coordinate change.

On the other hand, if coordinate change is *on* (i.e., `icoordchange=1` in `param.par`), the analysis is isotropic in the real space.

At 60° North, a degree E-W covers half the real distance of a degree S-N. On a graph scaled so that x and y are distances, the analysis is again isotropic (this is the desired effect). If you plot the same analysis with x and y axes equally spaced in degrees (as for the previous case), you will obviously get an ellipse (Fig. 8.5, left).

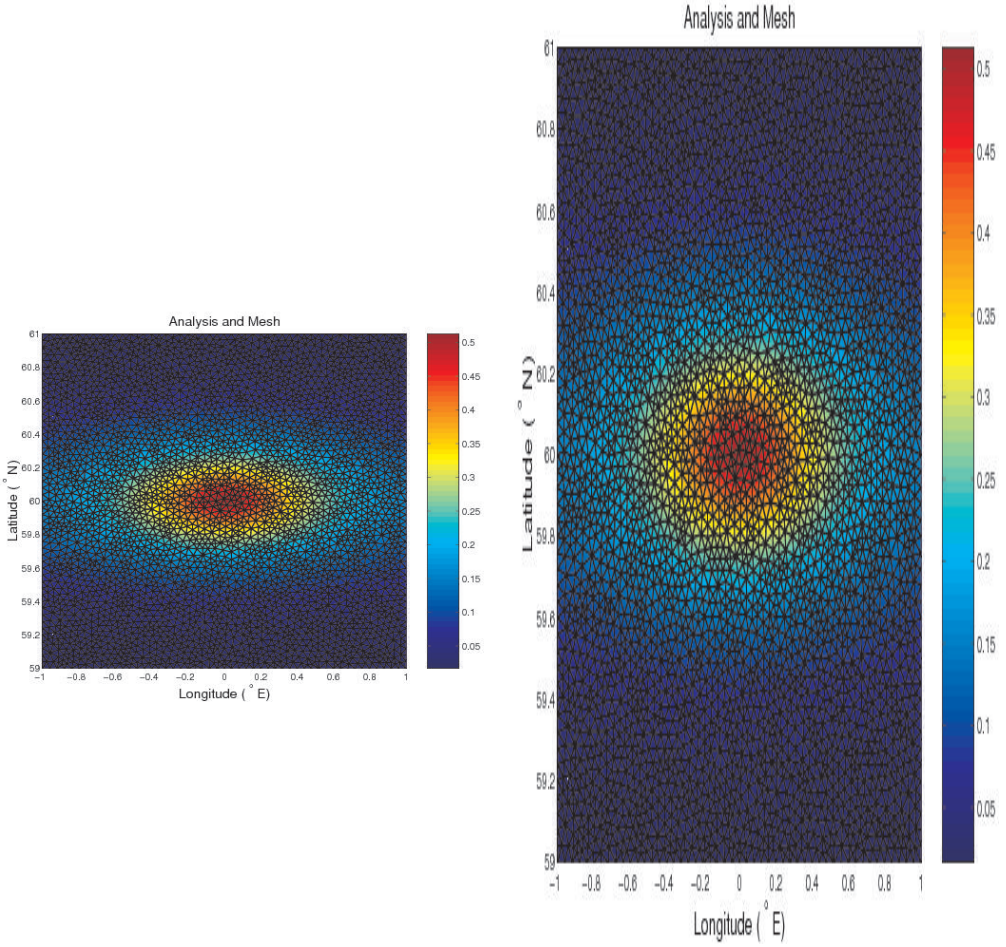


Figure 8.5: Analysis with coordinate change: the two figures represent the same field, but are drawn with different scales for the axes.

If we add an advection constraint characterized by $u = v = 1(m/s)$, the case with no coordinate change leads to a signal along the bisector (Fig. 8.6).

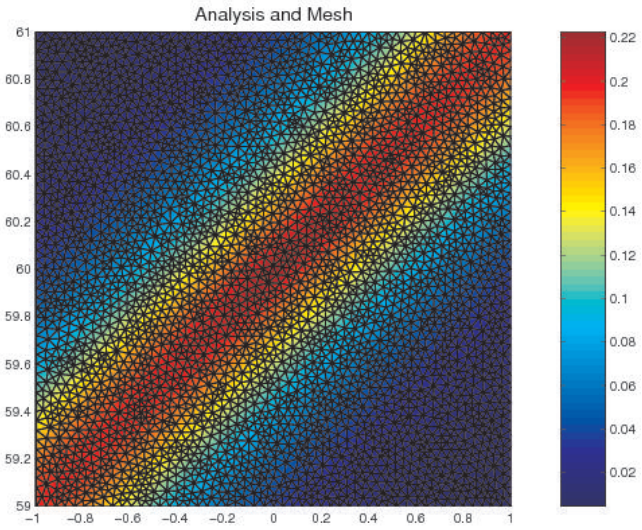


Figure 8.6: Analysis with advection but without coordinate change.

If coordinate change is activated, the advection direction in real space is not any more along the bisector in degrees, but in km (Fig. 8.7). Note that the advection constraint scales the overall velocity, so that a coordinate change does not change the intensity of the advection constraint, but only its direction.

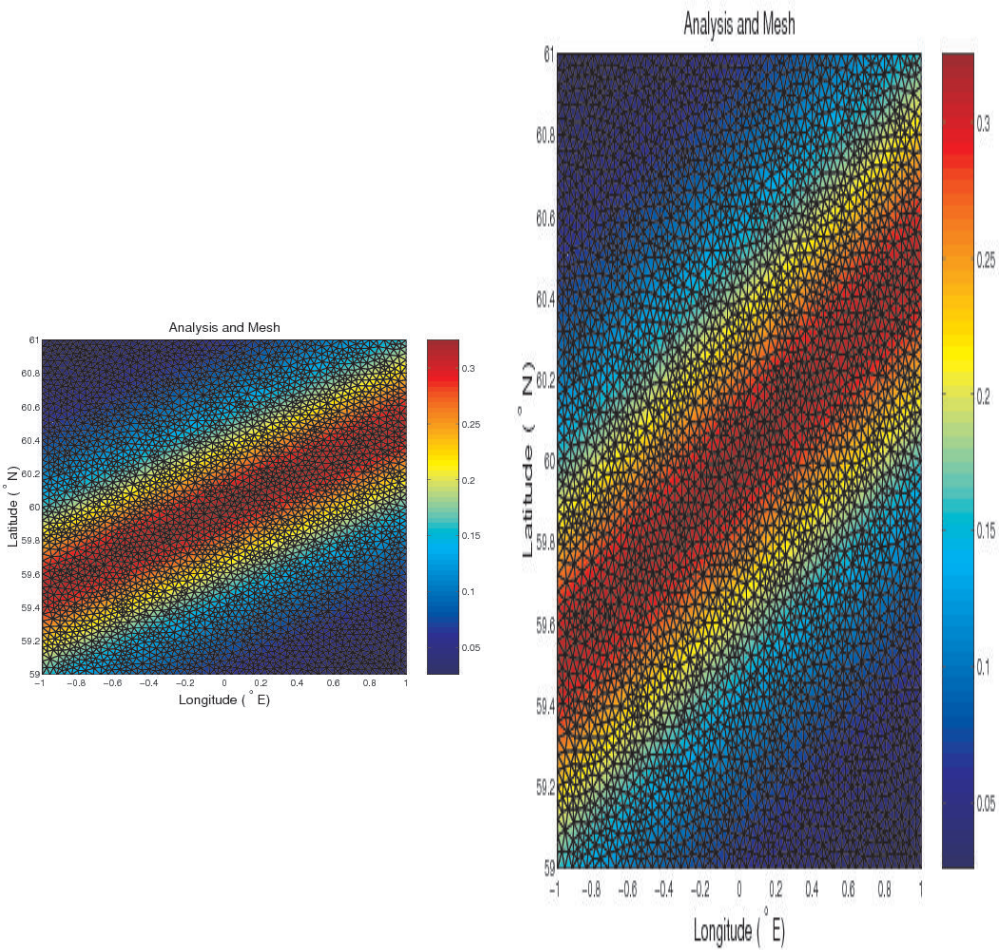


Figure 8.7: Analysis with advection and coordinate change.

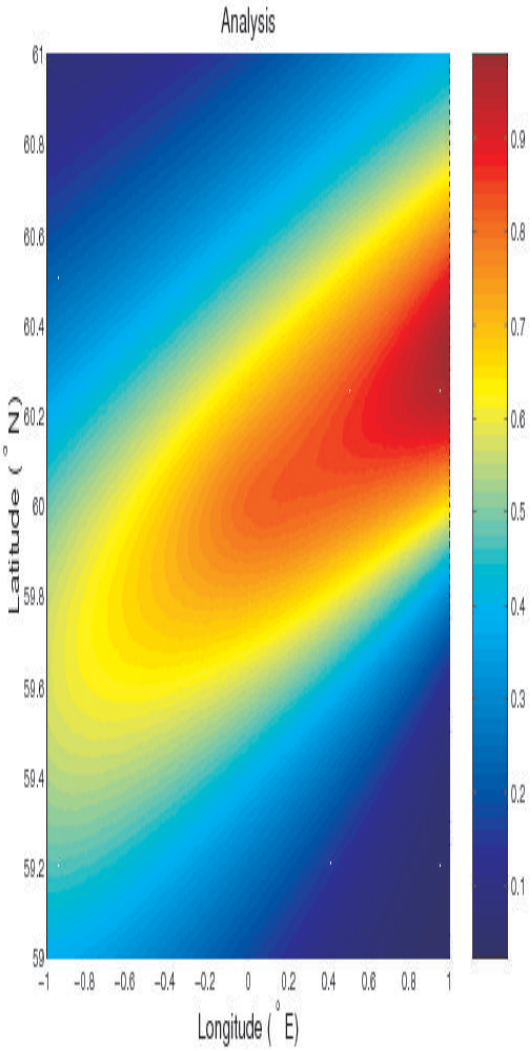


Figure 8.8: .

Note the diffusion coefficient is not changed. If this coefficient is given in Cartesian coordinates (in this case, it must be specified in m^2/s if velocities are in m/s) but you provide input in degrees and do not set `icoord=1`, the diffusion coefficient is basically overestimated by a factor 10^5.

For example, in the grid with `icoord=0` we can activate diffusion

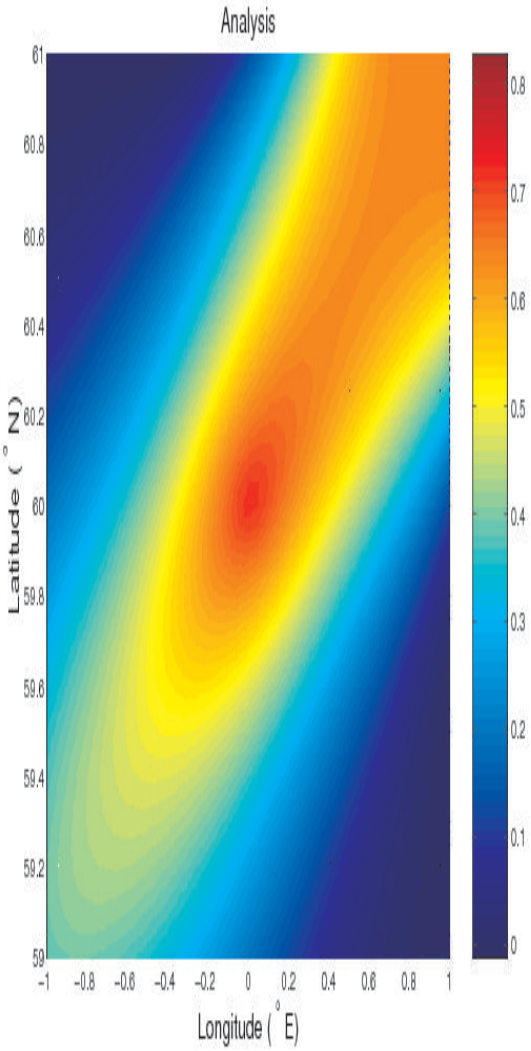


Figure 8.9: Diffusion coefficient divided by 110000 compared to the `icoord=1` *case.*

With no coordinate change, input values are taken as is. To recover a similar (but tilded and boundary modified) solution, we have to change manually the coefficient and divide by 110000 (degrees to meter scaling) so that the actual Reynolds number remains the same.

8.6 Summary: typical execution chains

8.6.1 Simple analysis

It is assumed that all the input files are already prepared and the parameters correctly assigned.

1. `divaload` your_directory
2. `divadress`
3. `divasave` your_directory

8.6.2 Analysis with evaluation of parameters

You start with correct data and contour file, but with parameters file that needs to be adapted.

1. `divaload your_directory`
2. `divafit -r` to compute the correlation length and replace its value in `param.par`;
3. `divagcv -r` to compute the signal-to-noise ration and variance of the background field, and replace them in `param.par`;
4. `divadress`
5. `divasave your_directory`

8.6.3 Analysis Relative Length (RL) Fields

To perform analysis using "variable correlation length" on the considered domain, one can provide the "Relative Length" field in the `input`.

"Relative Length" field can be produced by Diva on basis of data distribution using `divadacoverge`, or on basis of a mask netcdf file `mask.nc` provided in `input` using `dvncmask2RL`. The mask netcdf file must be written as shown in example 8.5.

An analysis using RL field based on a mask field provided in `input`, may be performed as follow:

1. `divaload your_directory`
2. `dvncmask2RL` to write `RL.dat` and `RLInfo.dat` in `input`;
3. `divadress`
4. `divasave your_directory`

```
netcdf mask
dimensions:
  lon = 100 ;
  lat = 100 ;
variables:
  float lon(lon) ;
  float lat(lat) ;
  float mask(lat, lon) ;
```

Example file 8.5: Header of mask netcdf file `mask.nc`.

9 POSTPROCESSING TOOLS

Various tools are available for visualization and processing of the gridded fields; some of them are presented in the following sections. It is up to the user to utilize his favourite drawing tools for representing the numerical results. Nevertheless, we provide several basic tools easily adaptable to facilitate the task.

Contents

9.1 Gnuplot

Gnuplot is a free portable command-line driven interactive data and function plotting utility, available for various platforms (http://www.gnuplot.info/). We provide some routines for plotting Diva inputs and outputs (data, contour, mesh, analysis etc) with the help of this tool. Running `divagnu` makes plots in png format.

Tips 9.1 *Plots provided by* gnuplot *are made to help the user to have a quick look at the results, immediately after the execution. However, these plots are not always suitable for publications or diffusion. The user is invited to create his own post-processing tools based on the examples provided in the next sections.*

Tips 9.2 *If you need larger fonts, on some systems they are available and you can edit the plotting program* `gnuwork\divaplotall` *and replace the driver definition by*

```
echo set terminal png transparent giant font system 14 size 1920,1540 crop \#ffffff >> bidon
```

Tips 9.3 *If you do not need all plots but only a few (eg. analysis, error and coastline) of them you can edit the plotting program* ***gnuwork\divaplotall*** *and replace the script line*
`for i in `ls diva_*``

by

```
for i in diva_analysis diva_error diva_coastline
```

9.1.1 Installation

gnuplotcan be easily downloaded for windows systems on the web page http://www.gnuplot.info. For Cygwin users, there are two possibilities:

1. you do not have X Windows System installed: in this case, it is advised to only install `wgnuplot`, available at
   http://downloads.sourceforge.net/gnuplot/gp422win32.zip for version 4.22.
   Once you have downloaded it, just unzip the folder in the location of your choice (provided it is located on the path of your system). The **gnuplot** window is activated either by typing `wgnuplot` in the Cygwin shell, or by creating a short-cut on your desktop to the executable `wgnuplot.exe`

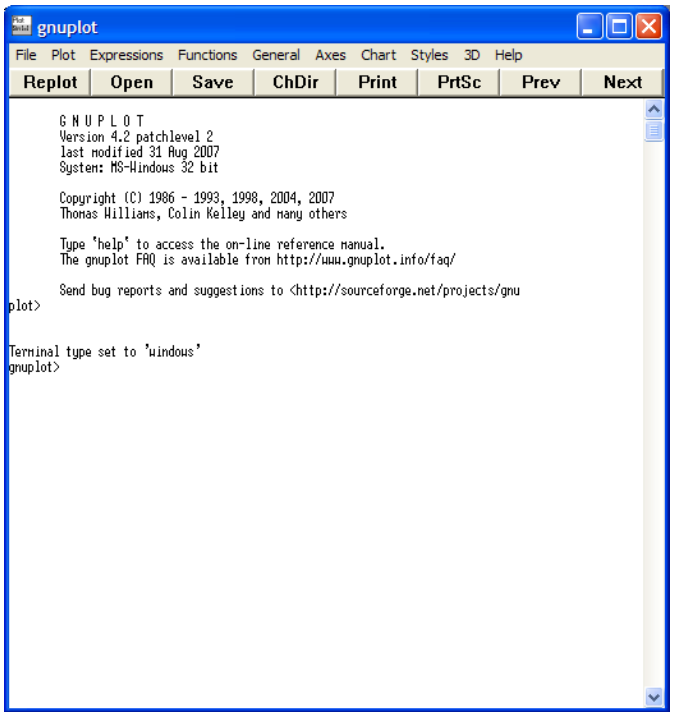


Figure 9.1: Gnuplot window.

2. X Windows System is already installed: run again the Cygwin `setup.exe` (for downloading and updating your Cygwin installation); in the "Select Packages" screen, look for the "Math" entry, select **gnuplot** and choose "'install". Once this installation is finished, **gnuplot** is launched from a XWin (obtained after typing `startx`) window by typing `gnuplot`.

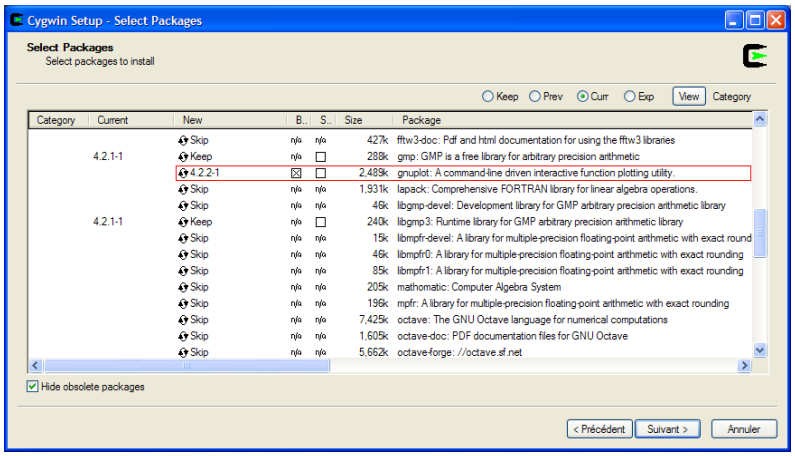


Figure 9.2: Installing **gnuplot** *with cygwin.*

9.1.2 Utilization

Normally Fortran sources (`forgnuplot*.f`) have been compiled during the Diva installation and executables placed into `DIVA3D/bin/`.

In directory `divastripped/gnuwork/`, edit `divaplotall` and adapt the header so that `gplot` indicates the correct path to your gnuplotexecutable.

Example

```
#=====================================================
# ADAPT the following to the gnuplot executable
gplot=/cygdrive/c/cygwin/usr/gnuplot/bin/wgnuplot.exe
#=====================================================
```

From `divastripped`, after running an analysis, type `divagnu`: this will create the figures in directory `gnuwork/plots/`. Note that `divagnu` will try to create all the possible figures, even if the corresponding script was not run, e.g., plot of outliers when no outlier detection was performed. This is why so many error messages are written on the screen, but you do not have to take them into account.

Here are some examples of plots created with gnuplot:

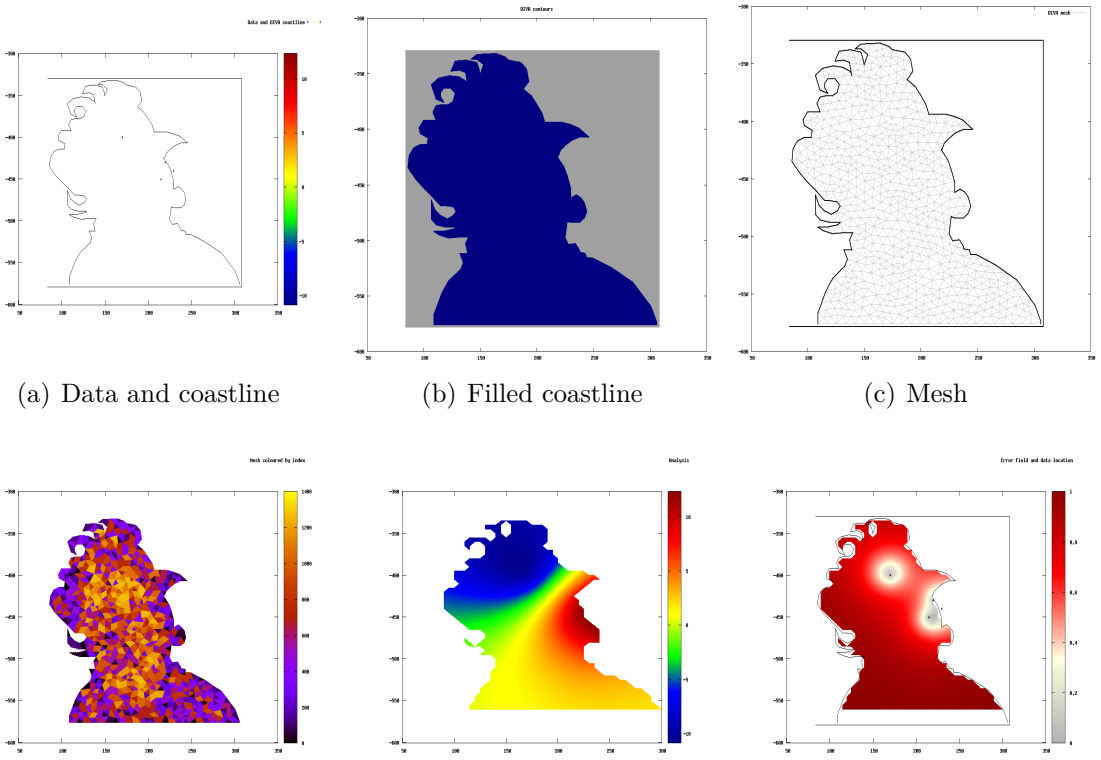
9.2 Matlab/ Octave

Tools to display contours, data, meshes, analysis and error fields are available at http://modb.oce.ulg.ac.be/mediawiki/index.php/Diva_matlab.

9.2.1 Installation

Download and extract the archives `Diva_matlab.tar.gz` and `matlab_example.tar.gz`

```
tar -xvf Diva_matlab.tar.gz
tar -xvf Diva_matlab_example.tar.gz
```



(a) Data and coastline (b) Filled coastline (c) Mesh

(d) Numbered mesh (e) Analysis (f) Error and data locations

Figure 9.3: Visualization with **gnuplot**.

In order to have the routines working properly, you need to install:

NetCDF toolbox, for reading the result files. For recent versions of Matlab, the routines for reading/writing NetCDF are readily available. For older versions, you can install it from http://mexcdf.sourceforge.net/downloads/.

m_map toolbox: optional but recommended, it allows one to plot generate various plots (mesh, data, analysis) using coastlines, projections etc (http://www.eos.ubc.ca/~rich/map.html).

9.2.2 Tools description

Table 9.1: Matlab programs for plotting. Set `mmapflag=1` if the m_map toolbox is installed. `valex` stands for exclusion value.

Routine	Mandatory input(s)	Optional input(s)	Utility
diva_contour.m	contourfile	mmapflag	Plot contour
diva_mesh.m	meshfile, meshtopofile	mmapflag	Plot mesh
diva_data_positions.m	datafile	dotsize, mmapflag	Plot data locations
diva_data.m	datafile	dotsize, mmapflag	Plot data values
diva_analysis.m	resultfile	valex, mmapflag	Plot the analyzed field

9.2.3 Examples of use

Open a Matlab session and set the path to the directory containing the function:

```
addpath('path_to_functions')
```

Define the input files:

```
exampledir   = path_to_example_directory;
contourfile  = [exampledir,'/coast.cont'];
datafile     = [exampledir,'/data.dat'];
meshfile     = [exampledir,'/mesh.dat'];
meshtopofile = [exampledir,'/meshtopo.dat'];
resultfile   = [exampledir,'/results.nc'];
```

Execute the different commands:

- Plot the contour:

  ```
  diva_contour(contourfile);
  ```

- Plot the finite-element mesh:

  ```
  diva_mesh(meshtopofile,meshfile);
  ```

- Plot the data positions:

```
diva_data_positions(datafile);
```

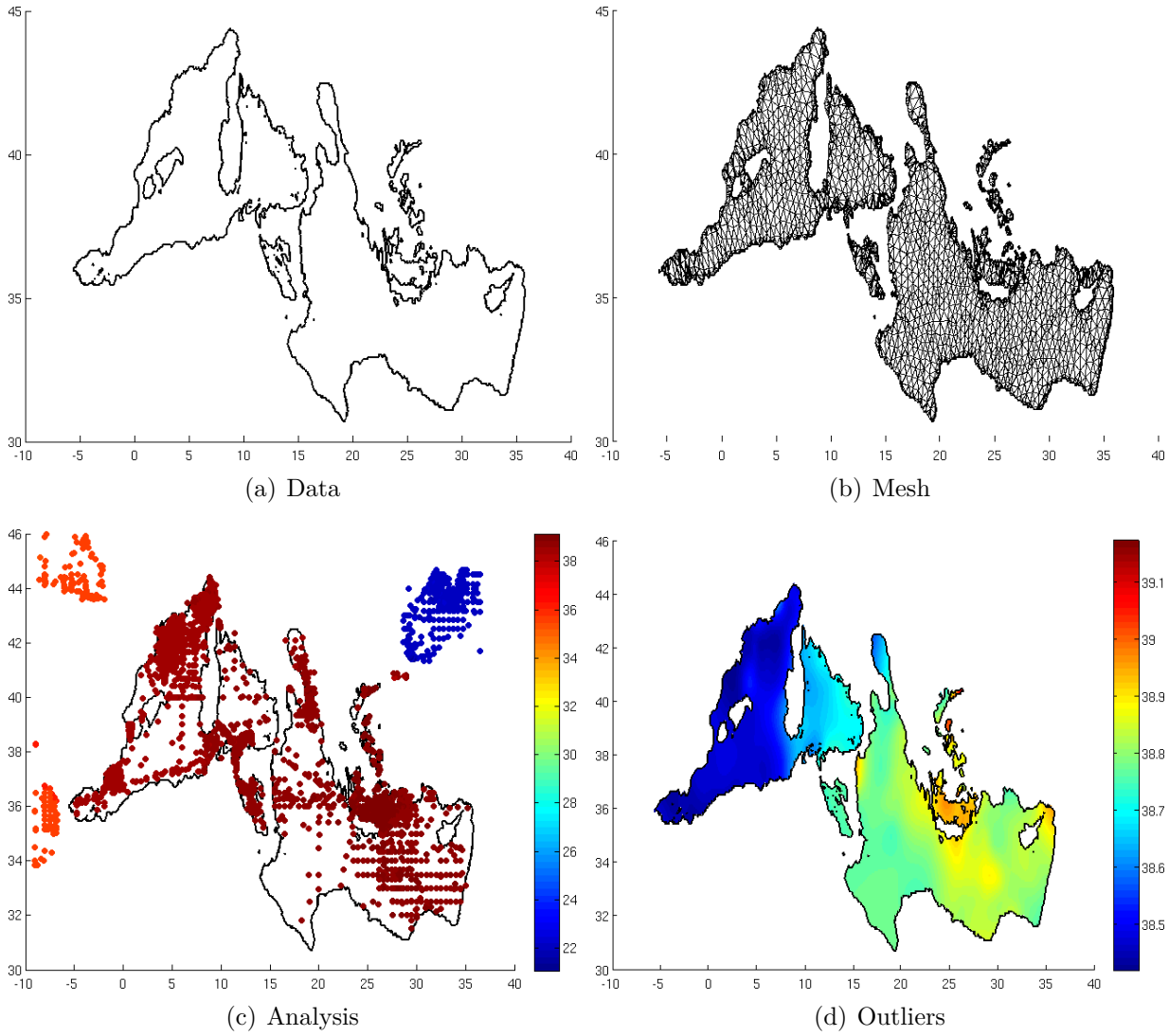
- Plot the data (with values):

```
diva_data(datafile);
colorbar;
```

- Plot the analysis:

```
diva_analysis(resultfile);
colorbar;
```

The resulting figures (without the m_map option) are shown below.



(a) Data (b) Mesh

(c) Analysis (d) Outliers

Figure 9.4: Examples of figures created with **Diva-Matlab** *toolbox.*

9.3 Python

Python (http://www.python.org/) is a object-oriented, free to use, programming language. It is directly available through the package manager of recent Linux distributions.

9.3.1 Installation

Download and extract the archive Diva_Python_tools_v1.0.tar.gz

```
tar -xvf Diva_Python_tools_v1.0.tar.gz
```

To have example files to test, extract the files from matlab_example.tar.gz (the same files used in the previous section) inside the python directory:

```
ctroupin@gher13 cd Diva_Python_tools_v1.0
ctroupin@gher13 tar -xvf Diva_matlab_example.tar.gz
```

Along with Python, it is necessary to install:

NumPy www.numpy.org, a package for scientific computing;

SciPy (http://www.scipy.org/), another package for science and engineering;

matplotlib (http://matplotlib.org/), a 2D plotting library, where one can find the basemap toolkit (https://pypi.python.org/pypi/basemap) particularly useful for plot data on map projection (somewhat equivalent to m_map in Matlab).

netcdf4-python (http://code.google.com/p/netcdf4-python/), the Python/numpy interface to netCDF.

Under Linux, the first three items are available with the package manager. The NetCDF interface requires a manual installation.

- Download the archive from http://code.google.com/p/netcdf4-python/downloads/list
- Check the *sha1 sum* and extract the archive:

```
ctroupin@gher13 ~/Software $ sha1sum netCDF4-1.0.4.tar.gz
cd1735a69446e558ba55034f184ee5f3d44d1a44  netCDF4-1.0.4.tar
   .gz
ctroupin@gher13 ~/Software $ tar -xvf netCDF4-1.0.4.tar.gz
ctroupin@gher13 ~/Software $ cd netCDF4-1.0.4/
```

- Follow the instruction written in file README:

```
ctroupin@gher13 ~/Software python setup.py build
ctroupin@gher13 ~/Software python setup.py install
```

9.3.2 Usage

Edit the files if necessary and run Python (either in a shell, or using a Python editor). An example of plots is shown in Fig. 9.5.

```
ctroupin@gher13 ~/ Diva_Python_tools_v1.0 python diva_plot_mesh
   .py
```

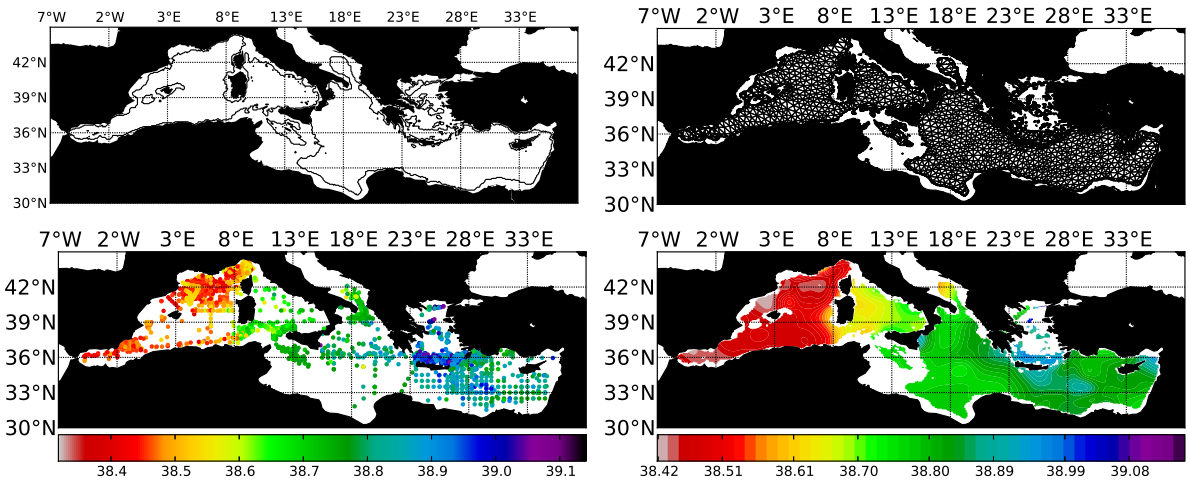


Figure 9.5: Examples of figures obtained with the Diva-Python toolbox.

9.4 General NetCDF visualization tools

NetCDF (network Common Data Form) format. It is an machine-independent format to represent scientific data. For more details, consult http://www.unidata.ucar.edu/software/netcdf/.

There are several tools that aim to provide a quick view of the content of a NetCDF files, such as the analyse and error fields provided by Diva. It is possible to export the results as a figure, but generally these software do not offer the possibility to customize the plots as could be done with the previous tools.

9.4.1 Ocean Data View

Among the numerous possibilities offered by ODV, there is a tool for accessing and visualizing local or remote NetCDF files (Schlitzer, 2012, Chapter 13).

9.4.2 NcBrowse

NcBrowse is available at http://www.epic.noaa.gov/java/ncBrowse/ and works with both Linux and Windows O.S.

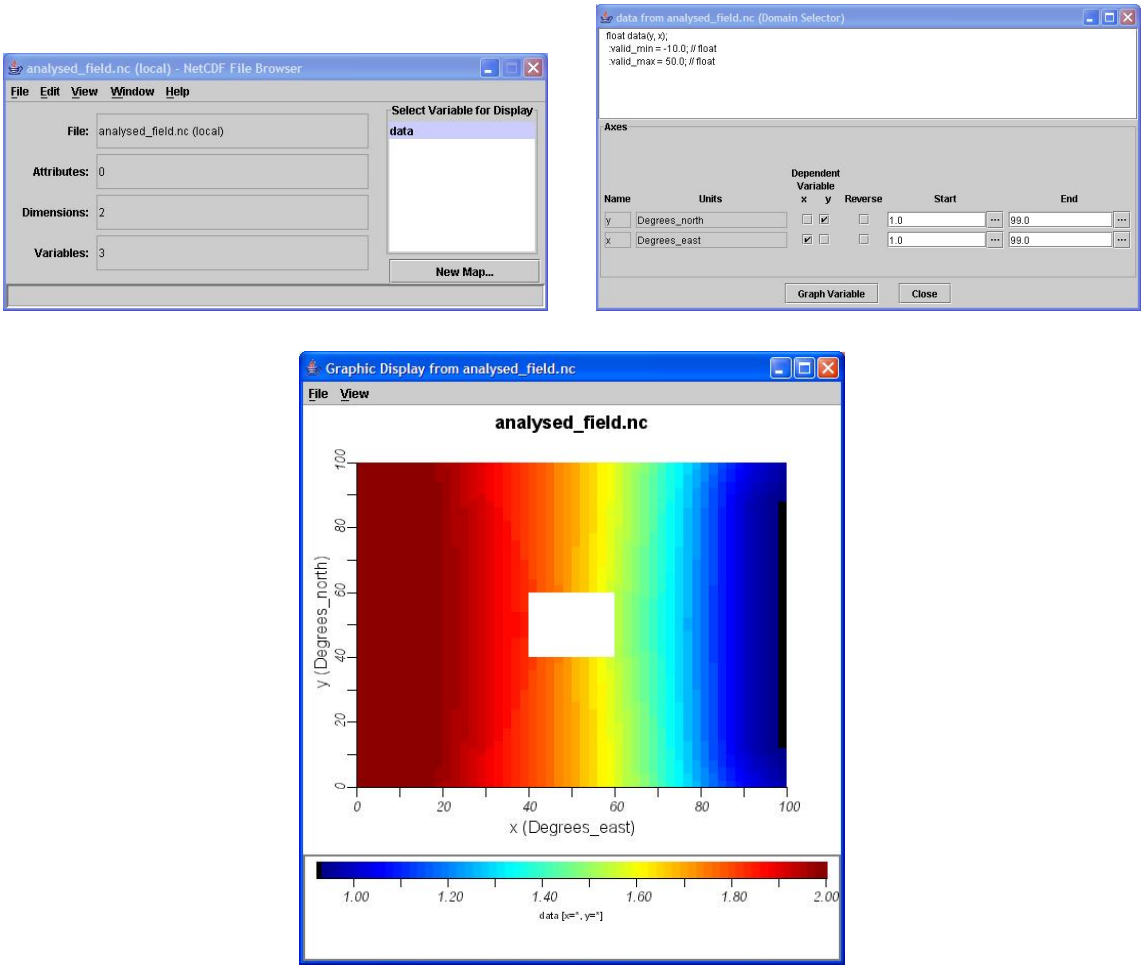


Figure 9.6: Plots of results with NcBrowse.

9.4.3 Ncview

Ncview (Linux and Windows + Cygwin) is available at
http://meteora.ucsd.edu/~pierce/ncview_home_page.html
but requires the NetCDF library to be compiled with your own system configuration.

Installation under Linux

Recent Linux distribution already permits the installation of Ncview through their package manager. Should it not be the case, the last version of Ncview is available here: ftp://cirrus.ucsd.edu/pub/ncview/ncview-2.1.2.tar.gz

Installation under Windows-Cygwin

Install and build the last NetCDF version for Unix: download the latest release and build as with Unix. The latest release is tested under Cygwin and passes all tests cleanly. To build under Cygwin, follow the Unix build instructions in a Cygwin shell. The `--enable-shared` option to configure will generate the `netcdf.dll`.

- Copy http://www.unidata.ucar.edu/downloads/netcdf/netcdf-3_6_2/index.jsp into directory of your choice
- Unzip the folder and type:

```
[Software]
./configure
...
make check..
...
make install
```

- download `Ncview` and unzip the folder
- type

```
[Software]
./configure
...
make
...
make install
```

- type `startx` (check if you have installed `Xfree`) and in the newly opened window, type
  `ncview name_of_the_file.nc`
- if the procedure is correctly followed, you should obtain windows similar to Fig. 9.7.

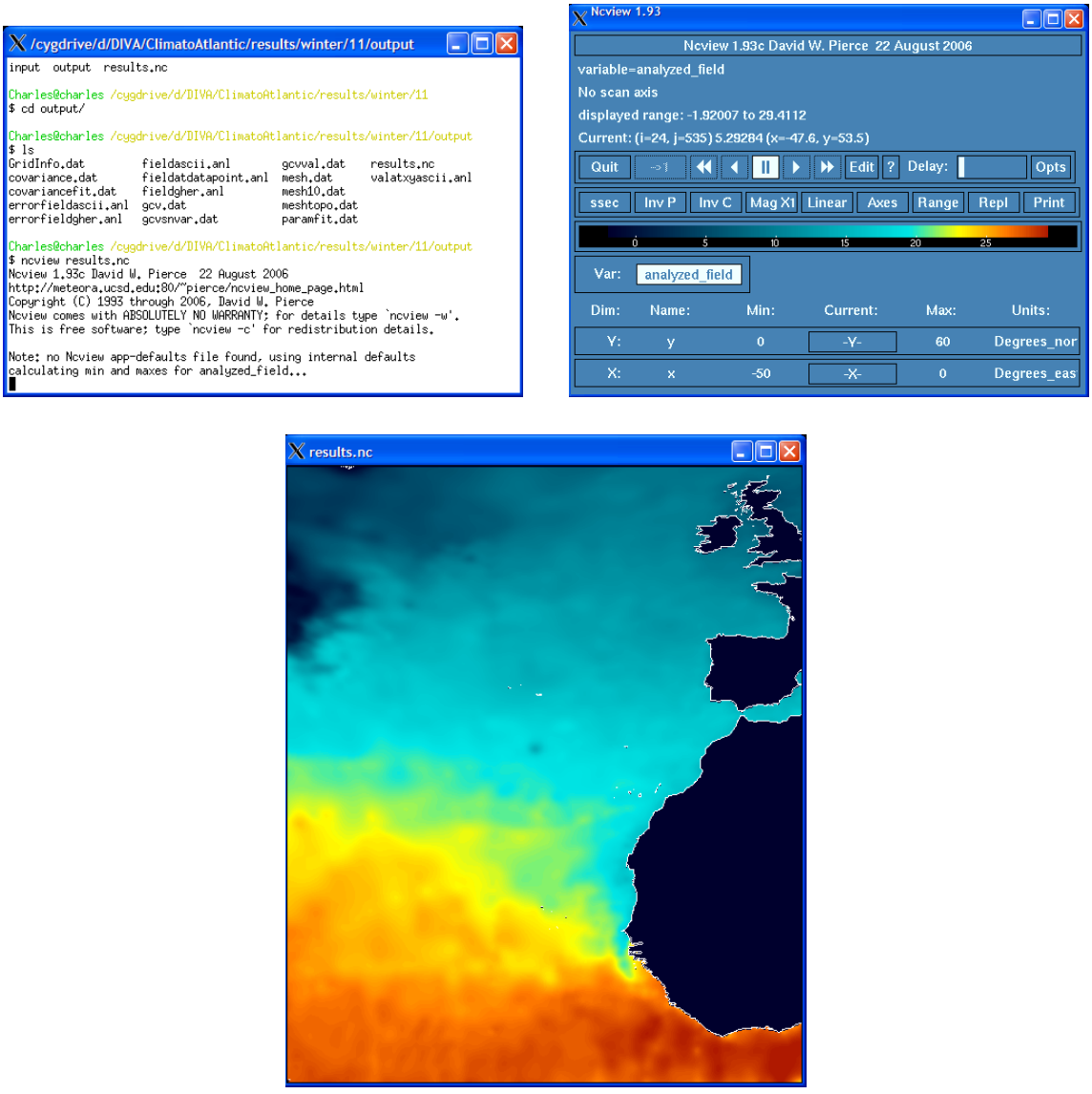


Figure 9.7: Plots of results with Ncview.

10 Realistic examples

A few examples with real data are described in this chapter. They can act as model for users who need to perform such kind of analysis.

Contents

10.1 Complete example

We present here a complete 2-D case treated in command-line. This example is taken from Troupin *et al.* (2012).

10.1.1 Preparation of the input files

To perform an analysis, you will need:

- a contour file (`coast.cont`),
- a data file (`data.dat`),
- a list of run parameters (`param.par`) and
- the locations of the points where you want to know the value of the analysed field (`valatxy.coord`).

Examples of these files are given in Chapter 6.

We recommend to create a new directory (let us call it `case1`) for each case you will treat and within this directory, two sub-directories name input and output. The four input files are then placed in `case1/input/`.

Let us assume that you created `case1` in `~/Examples/`. To copy them into the `diva-stripped/input/` directory, use the command:

```
bash-3.2$ divaload ../case1
```

Data

In this example we work with salinity measurements in the Mediterranean Sea at a depth of 30 m in September, for the 1980-1990 period (Fig. 10.1). The data set is built up by exploiting the SeaDataNet portal (http://www.seadatanet.org) and the World Ocean Database 2009 (WOD09, Boyer *et al.*, 2009) and contains 1061 data points.

Parameters

We start with the parameter file 10.1: the regular grid for the analysis extends from 7°W to 36°E and from 30°15'N to 45°45'N, with a horizontal resolution of about 10 km. The `icoordchange` parameter is set to 2, meaning that a cosine projection will be used for the coordinates.

```
# Correlation Length lc in km or degree??? according to param icoordchange
2
# icoordchange
2
# ispec (output files required, comments to come)
0
# ireg
2
# xori (origin of output regular grid, min values of X)
-7
# yori (origin of output regular grid, min values of Y)
30.25
# dx (step of output grid)
0.09
# dy (step of output grid)
0.0625
# nx max x of output grid
500
# ny max y of output grid
250
# valex (exclusion value)
-99
# snr signal to noise ratio
1
# varbak variance of the background field 2.5
1
```

Example file 10.1: First version of `param.par`

Contours

The land-sea contours are created from the GEBCO bathymetry. The Black Sea and the Atlantic Ocean were masked in order to concentrate only on the Mediterranean Sea properties.

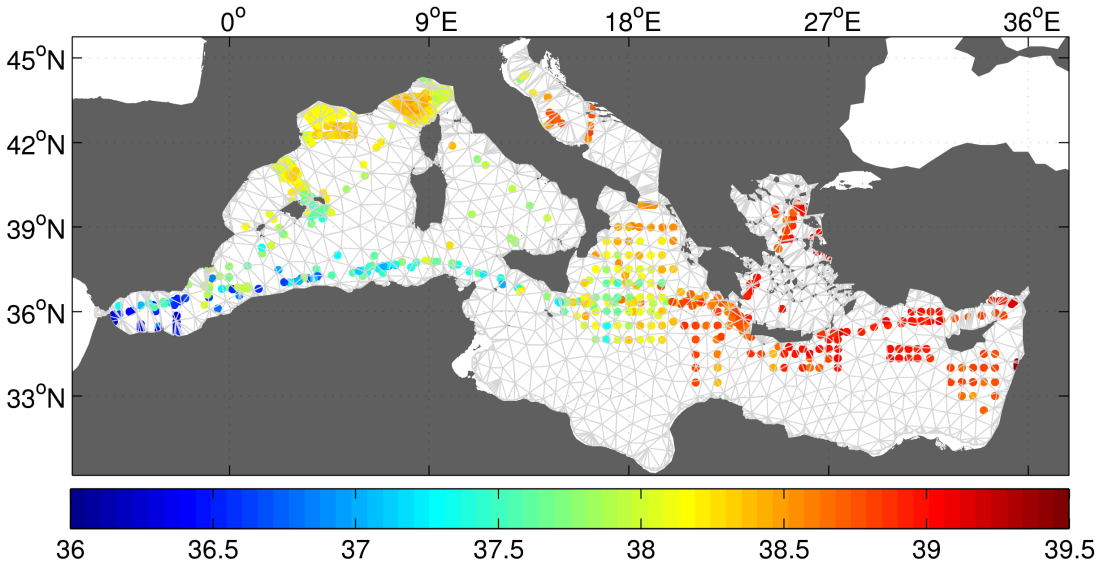


Figure 10.1: Finite-element mesh and salinity measurements used for the application.

10.1.2 Parameters determination

Correlation length

The toold `divafit` will provide a first guess of the parameters λ and L. It will generates the output files:

`covariance.dat`: contains distances between points, the covariance and the number of data couples used to estimate the covariance.

`covariancefit.dat`: contains the distance between points, the data-covariance and the fitted covariance.

`paramfit.dat`: contains estimates for the correlation length L and for the signal-to-noise ratio λ. You can manually replace the old values of λ and L in `param.par` by the new ones from `paramfit.dat`.

If you want the new L value to be automatically replaced, type

```
bash-3.2$ divafit -r
```

```
Correlation length
   1.3565110
 Signal to noise ratio
  0.72524220
 VARBAK
  4.59391139E-02
 Quality of the fit (0: bad 1: good)
  0.85546345970344528
 For information: correlation length in km is   151.44691
```

Example file 10.2: `paramfit.dat`

The fit yields the value $L = 1.36°$ ($\simeq$ 151 km).

10.1.3 Contour checking (optional)

If you want to check the contour file you want to use to generate the mesh, type `divacck`. The output `coast.cont.checked` is a thinned contour based on the length scale. Then simply copy the new contour into the `input` directory:

```
bash-3.2$ cp ./output/coast.cont.checked ./input/contour.cont
```

10.1.4 Mesh creation

Simply type `divamesh` to perform the mesh generation. All the parameters needed by Diva are contained in `coast.cont`, `param.par` and `coast.cont.dens` if you work with a

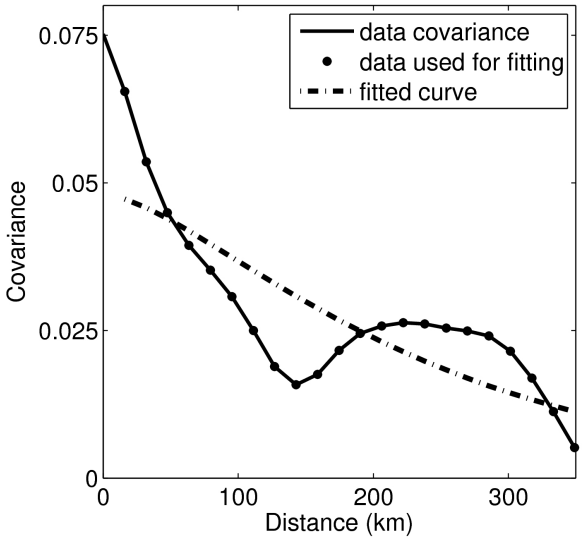


Figure 10.2: Fit of the data correlation to the theoretical kernel (dashed line).

non-uniform mesh. The mesh corresponding to this example is shown in Fig. 10.1. For the sake of visibility, the mesh was generated with a rather long characteristic scale: the correlation length was set to 3°, meaning the typical length of triangle edge is about 1°

10.1.5 Generalised Cross Validation

As described in Section 7.3, there are three tools to get an estimate of the signal-to-noise ratio: `divagcv`, `divacv` and `divacvrand`. For these tools to work, one has to provide an input file `gvcsampling.dat` (see example file 10.3) containing a list of values for the signal-to-noise ratio on which the estimator is tried.

```
0.1
0.3
0.6
1
3
6
10
30
```

Example file 10.3: `gvcsampling.dat`.

Estimated values for the parameters are given in `gcvsnvar.dat` (example file 10.4). You can then modify `param.par` (example file 10.5) according to these values before performing an analysis.

```
S/N S/N S/N
  30.00000     2.625988  3.359623
VARBAK VARBAK VARBAK
 0.1011484   7.5680271E-02 8.1069477E-02
```

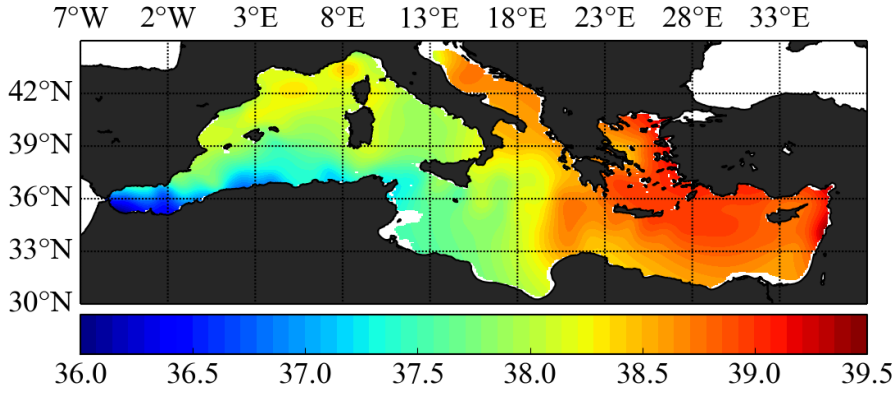
Example file 10.4: `gcvsnvar.dat` files obtained with `divagcv`, `divacv` and `divacvrand`.

```
# Lc: correlation length (in units coherent with your data)
1.3565110
# icoordchange
1
# ispec
3
# ireg
1
# xori: x-coordinate of the first grid point of the output
-10.0
# yori: y-coordinate of the first grid point of the output
30
# dx: step of output grid
0.2
# dy: step of output grid
0.2
# nx: number of grid points in the x-direction
236
# ny: number of grid points in the y-direction
81
# valex: exclusion value
-9999.0
# snr: signal to noise ratio of the whole data set
2.625988
# varbak variance of the background field
7.5680271E-02
```

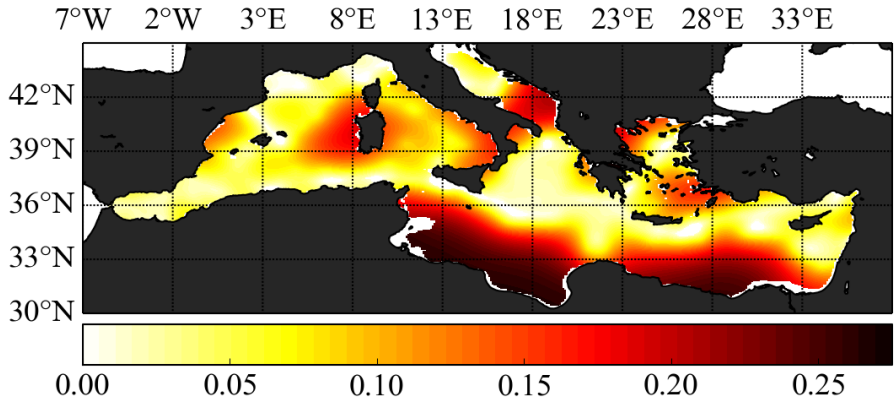
Example file 10.5: Adapted version of `param.par`

10.1.6 Analysis

Diva analysis is executed by typing `divacalc`. It not only provides the analysed field, but also the error field if `varbak` is not equal to zero. Results are presented in Fig. 10.3.



(a) Analysis



(b) Error

Figure 10.3: Analysed and error fields with $L = 1.36°$ *and* $\lambda = 2.63$.

10.2 Analysis of profiles from a cruise

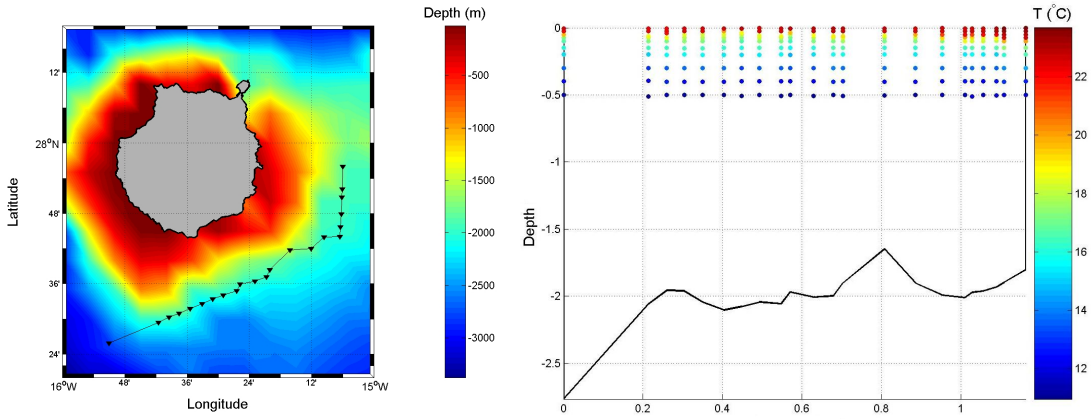
Usually Diva is used in horizontal planes and the coordinate system deals with longitude and latitude. One may also want to use Diva for interpolating data obtained during a campaign, i.e., several profiles along a determinate trajectory. In this case, the user will work in vertical planes: $x-$coordinate will be a (curvilinear) distance and y-coordinate will be the depth.

In horizontal planes, domains are physically limited by coastlines, while in vertical planes, the boundaries will be the sea surface and the bottom. The domain will be closed by artificial vertical lines, for example lines that originate from the first and last stations of the cruise (Fig. 10.4(b)).

We present hereinafter a complete example for this type of interpolation.

10.2.1 Creation of the contour

Generally the contour generation is easier in this case, since the transect cannot cross islands. Let us consider a transect that follows the track presented on Fig.10.4. The first step is to extract topography, which acts as a boundary of our domain. Methods for getting a topography are detailed in Section 7.1. For the horizontal axes, we worked with the distance computed with respect to the starting position of the cruise. Other choices are possible, i.e., degrees of longitude or latitude, distance from a reference point…



(a) Localization of the data (triangles) and topography of the region

(b) Data with limits of the domain

Figure 10.4: Contour generation.

10.2.2 Mesh generation

Since in physical oceanography, vertical length scales (100-1000 m) are much smaller than horizontal length scales (100-1000 km), an improvement is made if we take into account this anisotropy. To this end we need estimates of L_x and L_y, the horizontal and vertical length scales, respectively.

```
1
24
0.000000 0.000000
0.000000 -2.766513
0.213350 -2.058027
0.259753 -1.956031
0.303870 -1.960115
0.350149 -2.044557
...
1.108852 -1.895979
1.162687 -1.804136
1.162687 0.000000
```

Example file 10.6: Contour file of Fig. 10.4(b).

The most direct solution is to compute, for L_x, the mean distance between two stations, and for L_y, the mean distance between two measurements on a same profile. Then we compute the ratio

$$r = \frac{L_y}{L_x}$$

and multiply the horizontal coordinates by r. This allows one to work with the same length scale both on vertical and horizontal directions. With the data set from Fig. 10.4(b), we obtain:

$$\begin{aligned} L_x &= 4.4\,km, \\ L_y &= 55\,m, \\ r &= 0.0125. \end{aligned}$$

We then compute the length scale with the help of `divafit` and generate a new mesh, showed on Fig. 10.5.

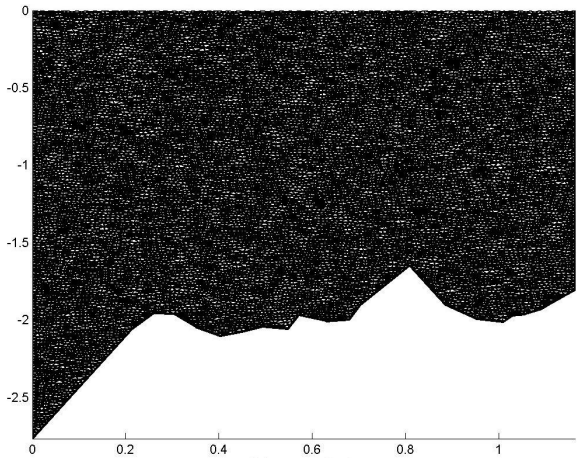


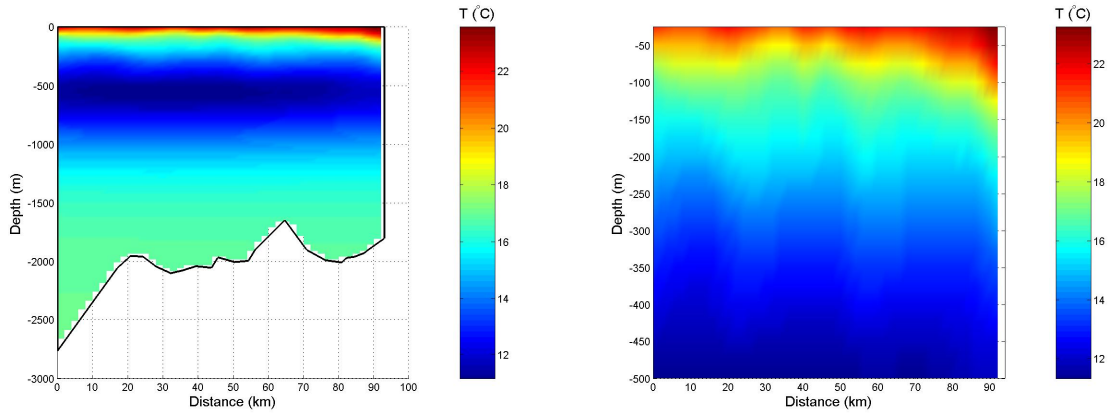
Figure 10.5: Mesh generated in the scaled domain.

Use of negative `icoordchange`

A more direct way to do the previous operation consists in changing the value of `icoordchange` in file `param.par`: by assigning a negative value to this parameter, we apply a scaling on the x coordinate (Sec. 6.2.3). In the present case we would put `icoordchange = -0.0125`. Then the classical Diva operations can be done.

10.2.3 Analysis

Once the mesh is created, the analysis is straightforward. The only thing to be aware of is the specification of the domain in file `param.par`: as we worked with scaled coordinates when generating the mesh, we have to do the same when specifying `x/yorigin` and `dx/y`. After the analysis, we may simply multiply the x coordinate by r to recover the original values. The results are presented on Fig. 10.6.



(a) Reconstructed temperature field

(b) Zoom between 0 and 500 m

Figure 10.6: Results of analysis.

10.3 Analysis of data from a transect

This case is very similar to the previous one. the difference is that here, data are collected along a trajectory of constant latitude.

10.3.1 Data

The track of the cruise (Fig. 10.7) follows a trajectory of constant latitude (24° N) across the Atlantic Ocean. Salinity for the year 1958 is represented on Fig. 10.8 along with the topography.

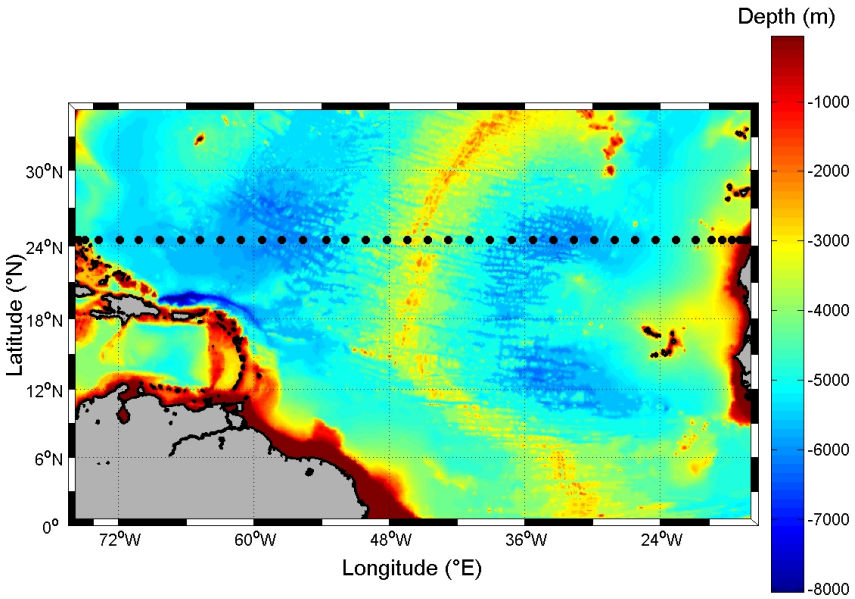


Figure 10.7: Transect stations (•) and bottom topography.

10.3.2 Contour creation

We have to convert degrees of longitude into kilometres to be coherent with the units, since the depth cannot be expressed in degrees. To this end, we used Matlab function `distance.m`, which calculates the *great circle distances* between two points on the surface of a sphere.

Extraction of topography

We extract topography with the help of Matlab function `m_tbase.m`, which uses 5−minute TerrainBase database. But any other source of topography suits.

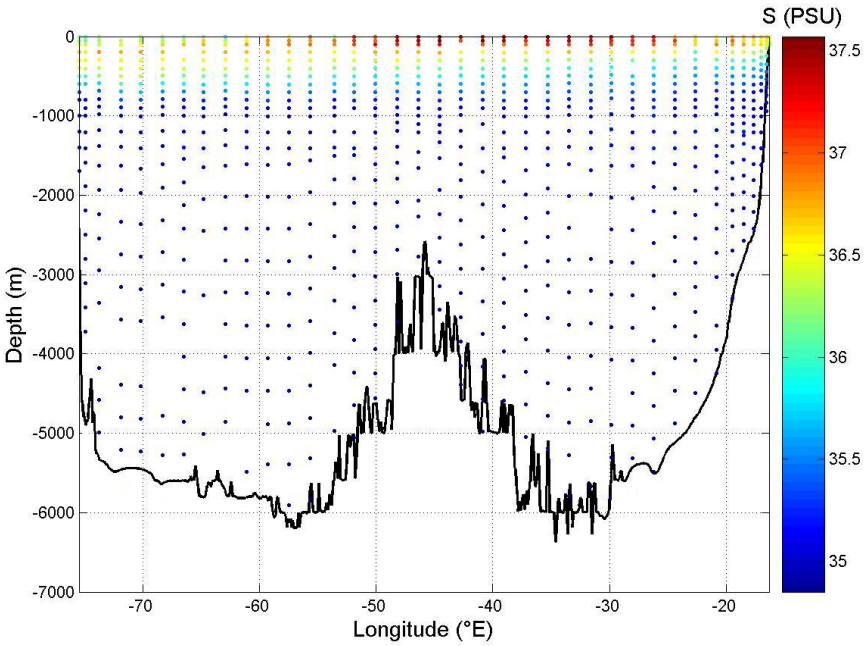


Figure 10.8: Domain and data.

10.3.3 Mesh

Computation of length scales

Similarly to the previous case, we compute horizontal and vertical length scales in order to take into account the domain anisotropy. Fig. 10.9 illustrates the difference between horizontal and vertical scales, as we represented the data within the domain with axes graduated in kilometres.

For L_x and L_y, the same definitions as in Section 10.2.2 are used. We find

$$\begin{aligned} L_x &= 156.76\,km, \\ L_y &= 204.40\,m, \\ \text{and the ratio } r &= 0.0013. \end{aligned}$$

Computation of correlation length

Correlation length is estimated with the help of `divafit`, which gives us:

$$L = 0.433\,km.$$

We generate the mesh (Fig. 10.10) with this value.

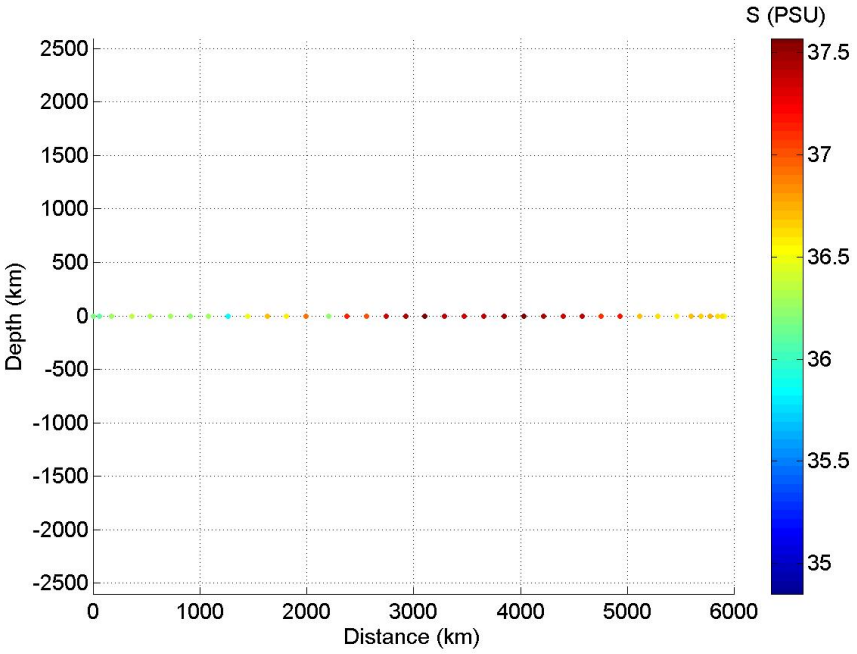


Figure 10.9: Data with axes in kilometres.

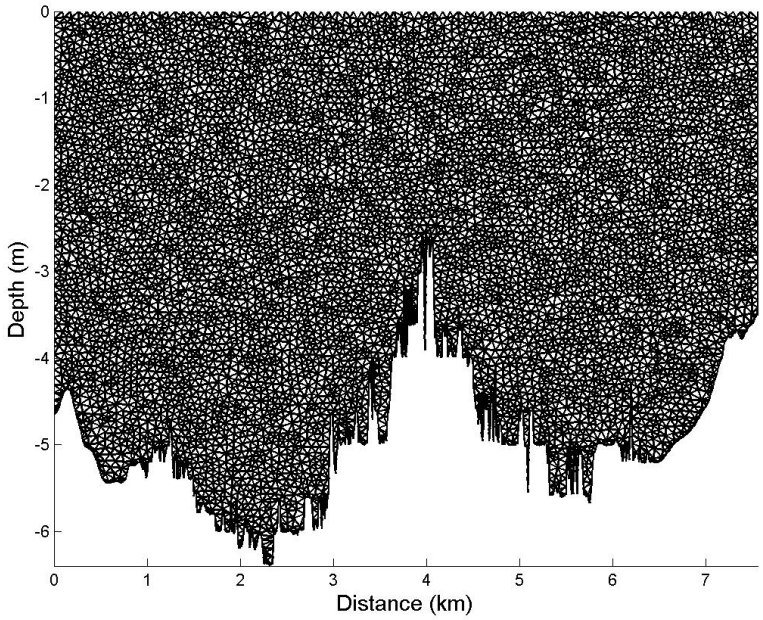


Figure 10.10: Mesh in the rescaled domain.

10.3.4 Analysis

Specification of the output grid

To be coherent with the scaling we made with the contour, we also have to consider scaled coordinates when specifying the output locations. Working in this coordinate system, we

carry out an analysis with the following values (in kilometres):

$$\begin{aligned} \texttt{xori} &= 0 \\ \texttt{yori} &= -6.0 \\ \texttt{dx} &= 0.01 \\ \texttt{dy} &= 0.002, \end{aligned}$$

which gives us a 809 $\times$ 299 point grid. Results are presented on Figs. 10.11 and 10.12

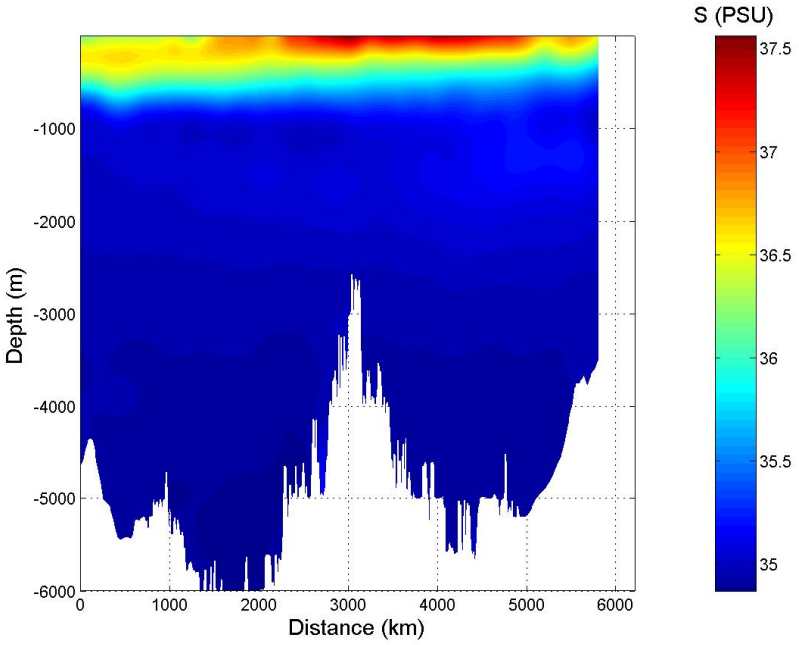


Figure 10.11: Analysed field.

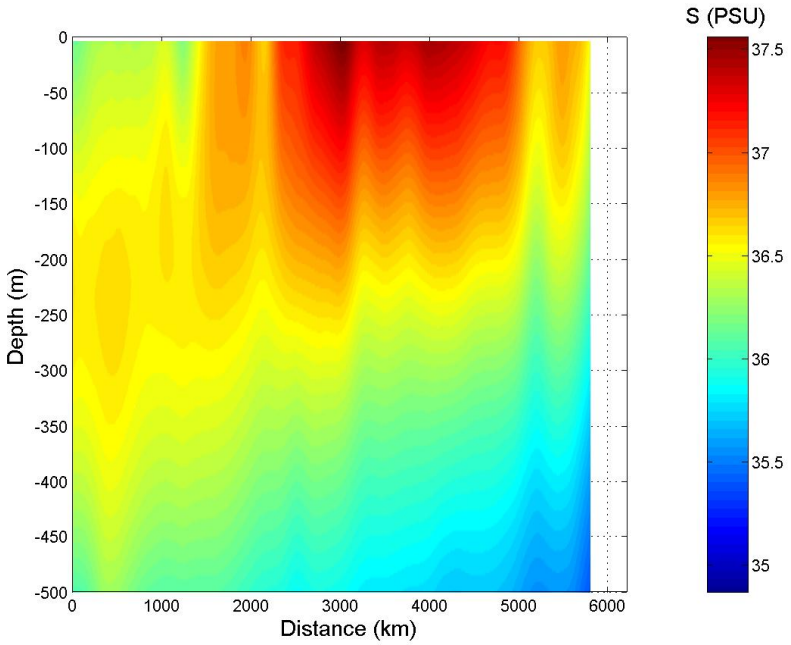


Figure 10.12: Analysed field between 500 m and sea surface.

10.4 Advection constraint: Mediterranean Sea

In this example, data points are located on a regular grid with alternate values of -1 and $+1$. An analysis with isotropic OI yields the field shown in Fig. 10.13: we obtain a pattern of alternating circular isolines on the whole domain (land is treated as it was sea). The analysis with Diva shows the influence of coastlines, as differences between the two cases are more obvious near coasts (Fig. 10.14).

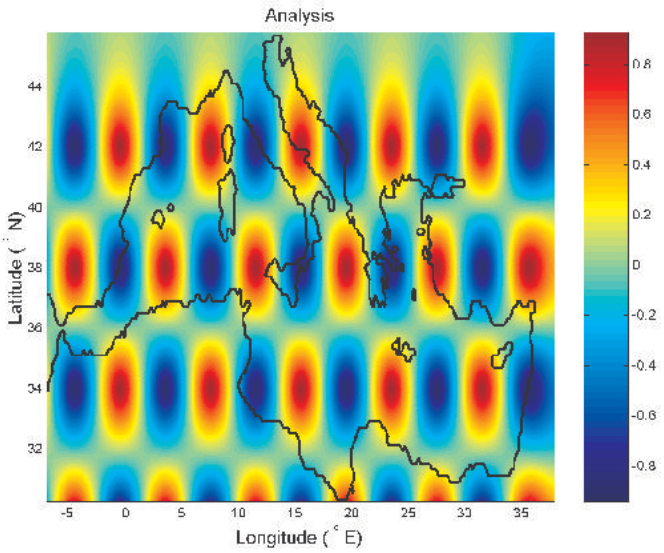


Figure 10.13: Isotropic OI.

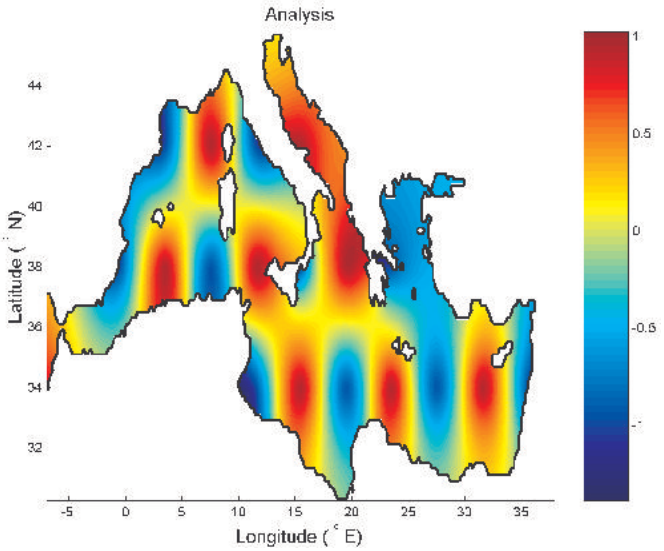


Figure 10.14: **Diva** *(with coastal effect).*

An illustration of the advection constraint is also presented: the velocity field is shown in Fig. 10.15 and the analysis produces the field of Fig. 10.16.

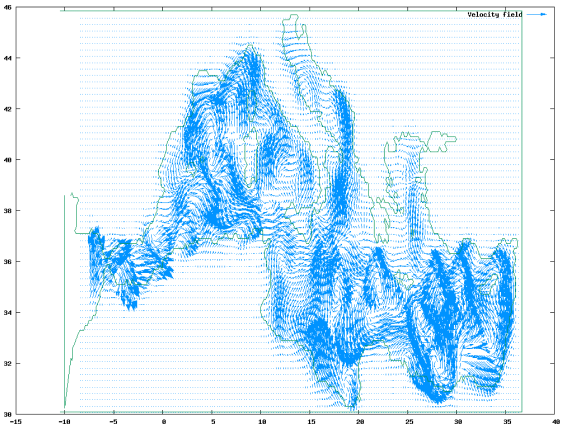


Figure 10.15: Velocity field used for the advection constraint in the Mediterranean Sea.

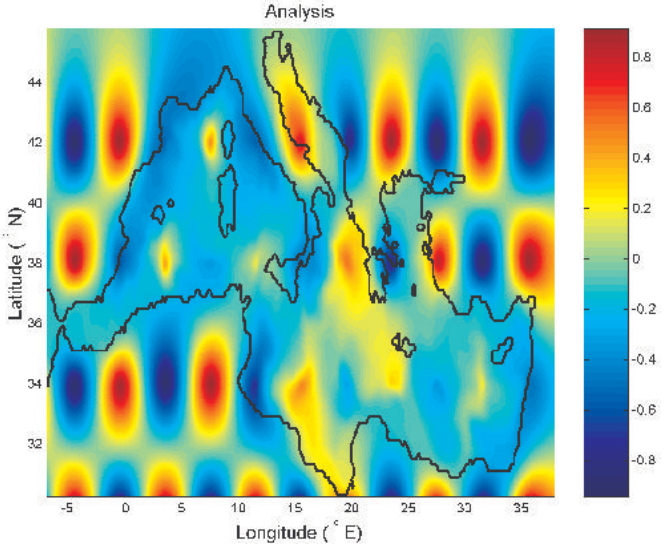


Figure 10.16: **Diva** *with advection (on full grid, no direct topography, but indirect via advection).*

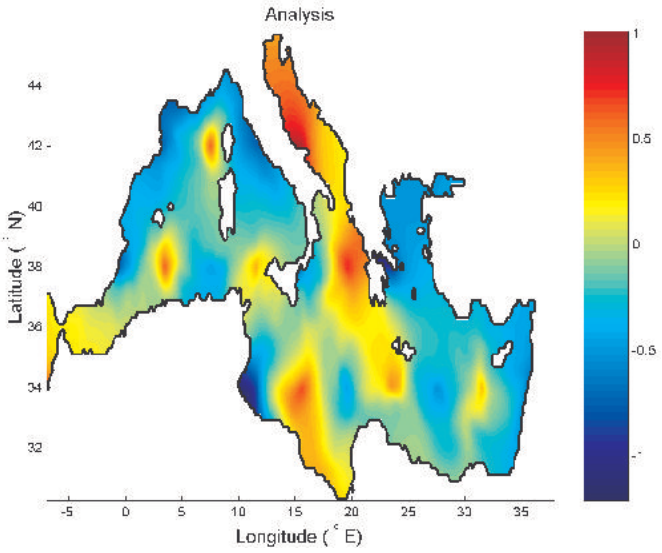


Figure 10.17: **Diva** *with topography and advection.*

11 Other implementations

In addition to the usual way of working with Diva (i.e., command line), there are other possibilities to use it without the installation of the whole code.

Contents

11.1 Diva-on-web

The idea behind Diva-on-web is to provide the possibility for the users to perform interpolations with Diva without having to install it on their machine. The web interface suits to a single analysis with a relatively low number of data. For climatologies, which requires the repetition of numerous analysis, the use of Diva is necessary.

The server is accessible at: http://gher-diva.phys.ulg.ac.be/web-vis/diva.html and a complete description of the interface is found in Barth *et al.* (2010).

11.1.1 Implementation

The web interface of Diva is based on OpenLayer (http://openlayers.org/) and is OGC-compliant (Open Geospatial Consortium, http://www.opengeospatial.org/). The server is a 2 quad-core Xeon E5420 running under Linux. The server and client software are available under GPL. The Web Map Server use `Python` language along with the plotting packages `matplotlib` (http://matplotlib.org/) and `basemap` (http://matplotlib.org/basemap/).

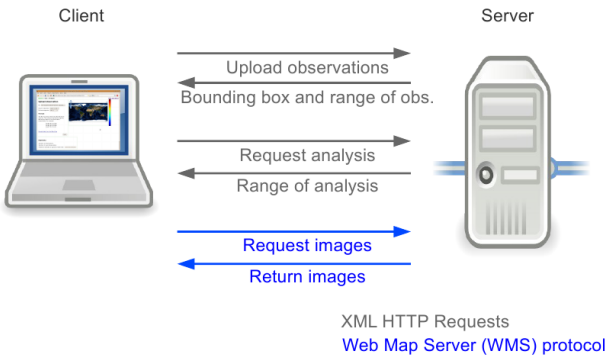


Figure 11.1: Communications between the server and the client for analysis with Diva-on-web.

11.1.2 A complete example

The steps to follow to obtain an analysed field is the following

1. Upload your data file (see Section 6.2.2 for the correct file format). (Fig. 11.2)
2. Define the analysis grid. (Fig. 11.3)
3. Select the analysis parameters. (Fig. 11.4)
   The script `divafit` provides an estimate for the correlation length (Fig. 11.5)
4. Perform the analysis. (Fig. 11.6)

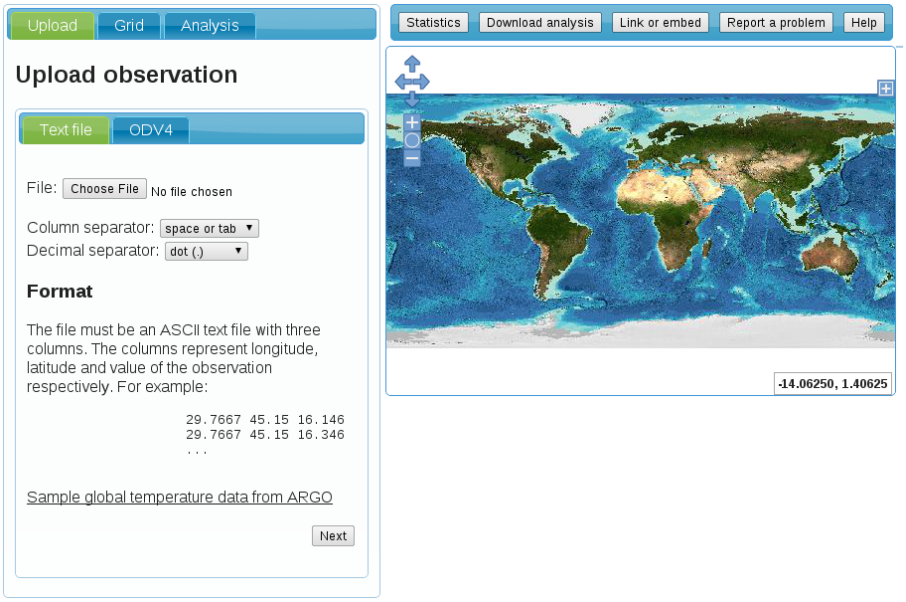


Figure 11.2: Upload of data.

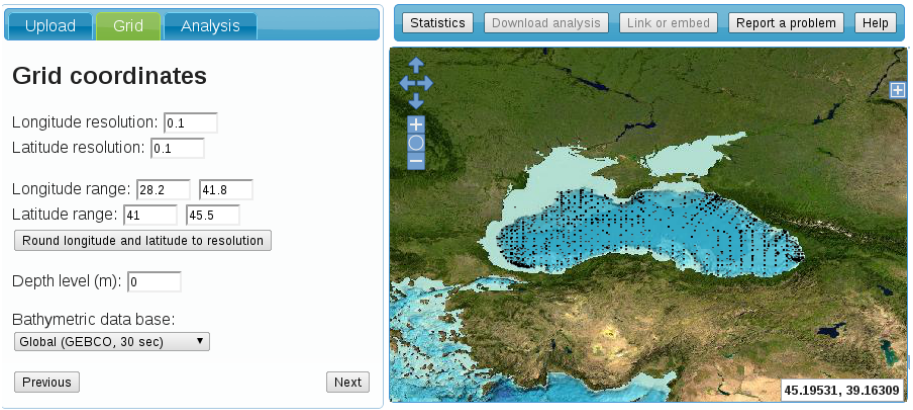


Figure 11.3: Grid coordinates.

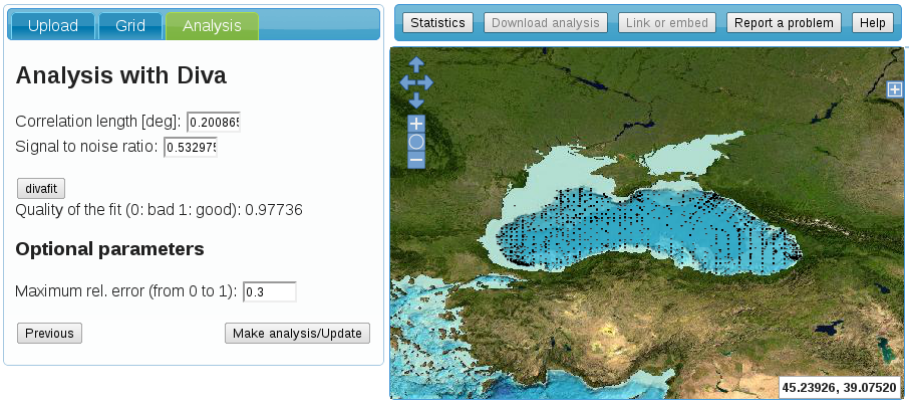


Figure 11.4: Parameters selection.

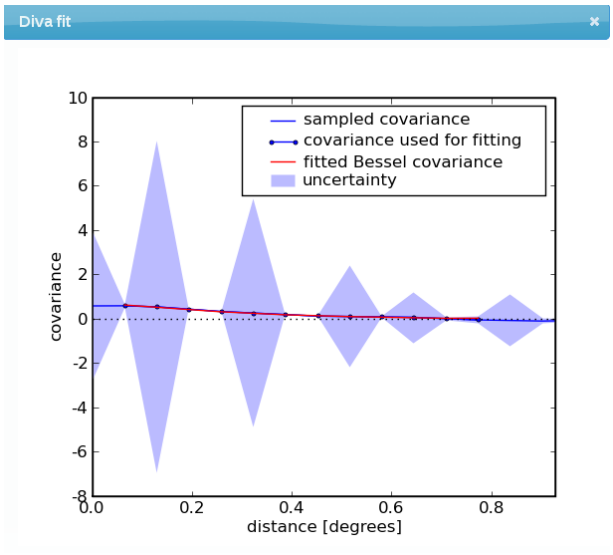


Figure 11.5: Visual results of `divafit`.

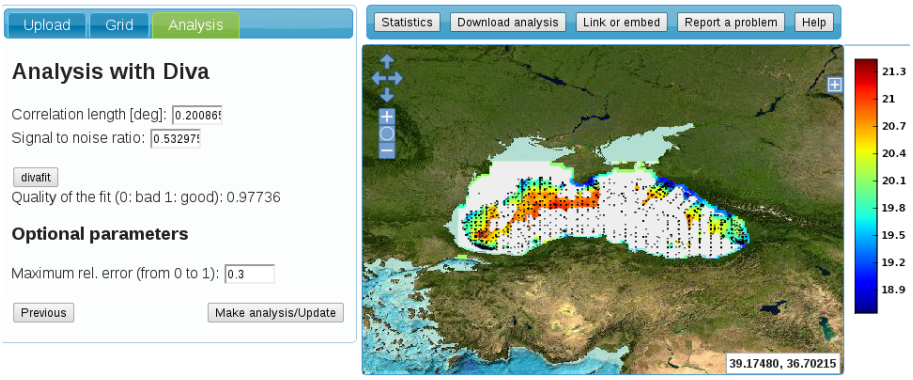


Figure 11.6: Analysis and mask based on relative error.

The outputs are available in various formats (Fig. 11.7): NetCDF, Matlab (or Octave) file, Keyhole Markup Language (KML) and other image formats.

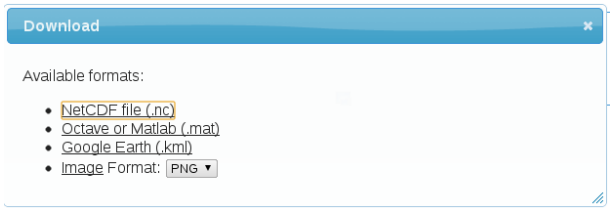


Figure 11.7: Exportation of the result field in different formats.

11.1.3 Conditions of use

- Open to all users without registration.
- CPU time and the number of observations is limited per user, in order to guarantee

availability to all. The current maximum CPU time is 10 minutes and the maximum number of observations is 100000.

11.2 Ocean Data View

Ocean Data View (ODV, Schlitzer, 2002) is a tool for the analysis and visualization of oceanographic data. Among the numerous possibilities ODV, we find the production of gridded fields based on the original data. Three methods are offered (Schlitzer, 2012):

1. *Quick gridding*, a weighted averaging algorithm optimized for speed, adapted for situations with millions data points.
2. *VG gridding*, a more sophisticated weighted averaging algorithm.
3. Diva gridding.

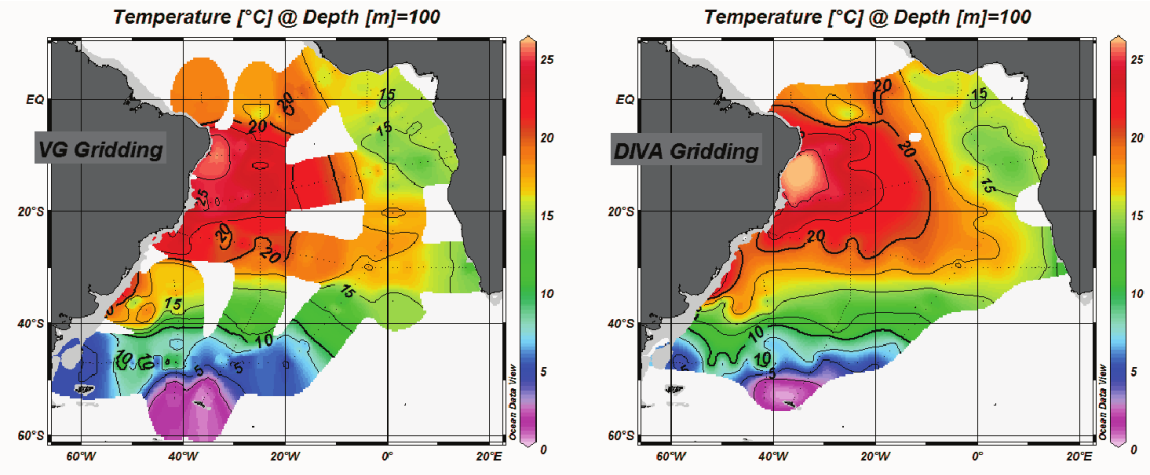


Figure 11.8: Example of VG gridding and Diva gridding with ODV (from Schlitzer (2012)).

Diva gridding is a simplified version of Diva implemented inside ODV, where the user can only modify a limited number of parameters.

11.3 Matlab toolbox

The Diva Matlab toolbox is an interface to perform 2-D analysis without having to compile the whole code and to type commands in a terminal.

11.3.1 Installation

Download the package from: http://modb.oce.ulg.ac.be/mediawiki/upload/divaformatlab.zip and unzip the archive:

```
[Software]$ wget http://modb.oce.ulg.ac.be/mediawiki/upload/
   divaformatlab.zip
...
[Software]$ unzip divaformatlab.zip
```

The structure is the following:

```
[Software]$ tree
.
|-- README
|-- divagrid.m
|-- linux_binaries
|   |-- contourgen.exe
|   |-- diva.exe
|   `-- generopt.exe
|-- testdivagrid.m
`-- windows_binaries
    |-- contourgen.exe
    |-- diva.exe
    `-- generopt.exe

2 directories, 9 files
```

The main file is `divagrid.m`, while `testdivagrid.m` provides a few example of how the function can be used. Directories `linux_binaries` and `windows_binaries`

11.3.2 Usage

The syntax `divagrid.m` is close to matlab `griddata.m` function, but has additional parameters.

To run Diva with matlab, `divagrid.m` has to be in the matlab path as well as the three executables:

- `contourgen.exe`
- `generopt.exe`
- `diva.exe`

figures (presented in diva workshop and SDN annual meeting

Part III

3-D analysis & climatology production (GODIVA)

Diva can be used to perform 3D-analysis for a given variable in an oceanic basin. In this case Diva tools are generally applied to successive horizontal layers at different depths of the basin. The resulting 2D-field analyses are gathered in 3D binary and NetCDF files.

The working directory to perform 3D-analyses is the same as for 2D-analyses: `diva-4.6.1/DIVA3D/divastripped`.

Contents

12.1 Input subdirectories

As described in Section 6.2, to perform a 2D-analysis, one needs to provide a set of input files in the `DIVA3D/divastripped/input/` directory. For 3D-analysis, the input files are provided in subdirectories of the input directory and in the input directory.

12.1.1 divadata subdirectory

In `DIVA3D/divastripped/input/divadata/` all the horizontal 2D data sets to be analysed are provided and named with regard to the variable name and the depth level number.

Convention: The files should be named as `var.1xxxx` where:

- `var` is for variable name.
- $xxxx$ is the level number and must be within the range $[0001, 9999]$.

Levels must be numbered from the bottom (lowest $xxxx$) to the top level (highest $xxxx$).

In this subdirectory, data density files related to data set files are stored:

`var.1xxxx.DATABINS` and `var.1xxxx.DATABINSinfo`.

Tips 12.1 *Density files are automatically generated when performing an analysis.* ■

12.1.2 divaparam subdirectory

In `DIVA3D/divastripped/input/divaparam/` are placed the `param.par` and `coast.cont` files, as well as all other input files related to Diva parametrisation. The `coast.cont` files are named following the corresponding level depth number. `param.par` files can be named following the corresponding variable name and the level depth number or only the level depth number:

Convention: The files should be named as:

- `coast.cont.1xxxx`
- `param.par` or `param.par.1xxxx` or `param.par.var.1xxxx`

$xxxx$ is the level number and must be within the range $[0001, 9999]$. Levels must be numbered from the bottom (lowest $xxxx$) to the top level (highest $xxxx$).

`input/divaparam/` content description

It may contain the following files:

`coast.cont.1xxxx`	`param.par`
`param.par.var.1xxxx`	`RL.var.1xxxx`
`RLinfo.dat`	`RL.dat`
`CLminmax`	`SNminmax`
`valatxy.coord`	`3Dconstraint`

`coast.cont.1xxxx`: files corresponding to the horizontal levels (as described in 6.2.1) can be automatically generated by Diva (see Section 12.3).

param.par.var.1*xxxx* files corresponding to the considered variable and horizontal levels (as described in 6.2.3) with optimised correlation length (L), signal-to-noise ratio (λ), and variance of the background ($VARBAK$) parameters can be automatically generated by Diva from a generic `param.par` file placed in `DIVA3D/divastripped/input/` (see Section 12.3).

RL.var.1*xxxx***:** files (and the related info file `RLinfo.dat)` can be placed in the `input/divaparam/` if one wants to use relative correlation length. They can be also automatically generated by Diva (based of data distribution). It is also possible to place only a unique file named `RL.dat` to be used for all the levels.

3Dconstraint is a two-column file, where each line corresponds to the level of the same number, and contains the two constraint parameters to be used (see Section 8.5) when performing analysis with advection constraint.

The advection constraint files are placed in the `input/divaUVcons` subdirectory. One can provide files named with regard to the variable and the level to which they correspond: `Uvel.var.`1*xxxx*, `Vvel.var.`1*xxxx*, or only to the level: `Uvel.`1*xxxx*, `Vvel.`1*xxxx*. Default files `Uvel.dat`, `Vvel.dat` and `UVinfo.dat` may be placed to be used for levels for which related (advection) files are missing.

CLminmax, and/or SNminmax can be placed in the `divaparam` subdirectory. These files are used (if present) for L and/or λ optimisation, in the case where the maximum and the minimum acceptable values for correlation length, and/or signal-to-noise parameter values for each level is to be specified (see Section 12.3).

valatxy.coord.var.1*xxxx* **files:** two-column (at least) lists of locations where one wants to have the performed analysis values in ascii files as an output for the related variable and level. It is possible to provide files `valatxy.coord.`1*xxxx* for the corresponding levels only, independently of the variable and only `valatxy.coord` independent from variables and levels. The output will be always related to variables and levels.

12.1.3 More input subdirectories

The directory `DIVA3D/divastripped/input/` may also contents other subdirectories, as described below.

divaUVcons

This subdirectory is located in the `divastripped/input` directory, and contains input files of advection constraint.

It may contain the following files:

`UVinfo.var.`1*xxxx*	`UVinfo.`1*xxxx*	`UVinfo.dat`
`Uvel.var.`1*xxxx*	`Uvel.`1*xxxx*	`Uvel.dat`
`Vvel.var.`1*xxxx*	`Vvel.`1*xxxx*	`Vvel.dat`

Uvel.var.1*xxxx*, **Vvel.var.**1*xxxx* **and UVinfo.var.**1*xxxx* named with regard to the variable name and the corresponding level depth number, and/or

Uvel.1*xxxx*, **Vvel.**1*xxxx* **and UVinfo.**1*xxxx* numbered following the level to which they correspond and/or

Uvel.dat and Vvel.dat and UVinfo.dat .

divarefe

This subdirectory is located in the divastripped/input/ directory, and contains reference field files which can be used by Diva as background for the analyses. This files can be semi normed reference field files produced previously by Diva.

It may contain the following files:

GridInfo.dat	var.1*xxxx*.ref
var.1*xxxx*.ascii.ref	var.1*xxxx*.datapoint.ref

var.1*xxxx***.ascii.ref:** 2D gridded reference field files in ascii format named with regard to the corresponding variable name and depth level number, and/or

var.1*xxxx***.ref:** 2D gridded reference field files in GHER format (binary) named with regard to the corresponding variable name and depth level number, and if available

var.1*xxxx***.datapoint.ref:** data file (three columns files) which contains the variable reference field value at data points.

divamesh

This subdirectory is located in the divastripped/input directory, and contains mesh files which can be used by Diva instead of generating a new ones. This files can be produced previously by Diva in a preprocessing step .

It may contain the following files:

meshtopo.1*xxxx*	mesh.dat.1*xxxx*

meshtopo.1*xxxx* **and related mesh.dat.**1*xxxx* , named following the depth level number to which they correspond.

12.2 Input info files: contour.depth & 3Dinfo

In order to use the three dimensional features of Diva, one has to provide two info-files in the DIVA3D/divastripped/input/ input directory:

contour.depth 3Dinfo

12.2.1 contour.depth

contour.depth contains a list of depth values (one value per line) of the considered levels. The first line corresponds to the **deepest** level and the last one to the **top** level.

3Dinfo is the file where shell script reads the parameter values for the 3D execution: variable name, levels to be treated, flags values controlling the execution of tasks to be performed and, maximum and minimum acceptable values for correlation length (L) and signal-to-noise (λ) parameters. If one desires to specify the maximum and the minimum values for L and/or (λ) parameter for each level, a file `CLminmax` and/or `SNminmax` must be placed in the `divaparam` subdirectory. In this case the corresponding maximum and minimum values in the `3Dinfo` file are ignored.

```
2000
1500
1000
800
600
500
400
300
250
200
150
125
100
75
50
30
20
10
5
0
```

Example file 12.1: contour.depth

12.2.2 The 3Dinfo file

The information file `3Dinfo` must be placed in the `input` directory and must contain all the following information and option flag values:

- *var* : variable short name which names data files (`var.1`$xxxx$)
- L_1 : Number of the first level to be treated.
- L_2 : Number of the last level to be treated.

- **contour generation** :
  * = 1 if contour files are to be generated,
  * = 2 if advection constraint (anisotropic correlation along topography) files are to be generated from `topo.grd`,
  * = 3 if contour files and advection constraint are to be generated.
- **Cleaning data and Relative Length**:
  * = 1 if data files are to be cleaned,
  * = 2 if relative length files are to be generated,
  * = 3 if data files are to be cleaned and relative length files are to be generated.
  * = 4 if outliers are to be cleaned from data files.
  * = 5 if outliers are to be cleaned from data files and, relative length files to be generated.
- **Parameter optimization**: Possible flag values are 0, 1, 2, 3, -1, -2, -3, 10, -10, 30 and -30:
  * = 1 if correlation length parameters are to be estimated,
  * = 2 if signal-to-noise ratio (λ) parameters are to be estimated,
  * = -1 if correlation length parameters are to be estimated and vertically filtered,
  * = -2 if signal-to-noise ratio (λ) parameters are to be estimated and vertically filtered,
  * = 3 if both correlation length and signal-to-noise ratio parameters are to be estimated,
  * = -3 if both correlation length and signal-to-noise ratio parameters are to be estimated and vertically filtered,
  * = 10 if correlation length parameters are to be estimated using data mean distance as a minimum,
  * = -10 if correlation length parameters are to be estimated using data mean distance as a minimum and vertically filtered,
  * = 30 if both correlation length and signal-to-noise ratio parameters are to be estimated using data mean distance as a minimum (for L),
  * = -30 if both correlation length and signal-to-noise ratio parameters are to be estimated using data mean distance as a minimum (for L), and both parameters vertically filtered.
- **Perform analysis**: Possible flag values are 0, 1 and 2:
  * = 2 if semi normed reference fields of the considered variable are to be performed for all the levels between L_1 and L_2.
  * = 1 if analysis fields of the considered variable are to be performed for all the levels between L_1 and L_2.

- $MaxCL$: maximum value for correlation length (ignored if a `CLminmax` file is provided in `divaparam`).
- $MinCL$: minimum value for correlation length (ignored if a `CLminmax` file is provided in `divaparam`).
- $MaxSN$: maximum value for signal-to-noise ratio (ignored if a `SNminmax` file is provided in `divaparam`).
- $MinSN$: minimum value for signal-to-noise ratio (ignored if a `SNminmax` file is provided in `divaparam`).
- $Gnplt$: $= 1$ if Gnuplot plot files are to be generated.
- $MinGP$: minimum value of the variable for Gnuplot plots.
- $MaxGP$: maximum value of the variable for Gnuplot plots.
- *'Title String' : Title string for 3D-NetCDF file.*
- *'Variable name string' : Variable long name string.*
- *'Units string' : Variable units string*

```
# Variable (var) to be analysed (located in data/var.1xxxx):
psal
# Number of the first level to be processed (bottom?):
1
# Number of the last level to be processed (surface?):
25
# Contours generation (0, 1, 2, 3):
3
# Data cleaning (0: if no, 1: data cleaning only, 2: RL files, 3: 1 and 2):
3
# Parameters optimisation (0, 1, 2, -1, -2, 3, -3, and +or- 10,20 and 30):
-30
# Perform analyses (0 if no, 1: analyses, 2: references):
1
# Minimum value for correlation length:
0.5
# Maximum value for correlation length:
4.
# Minimum value for S/N:
0.1
# Maximum value for S/N:
50.
# Gnuplot plots generation (1 if yes, 0 if no):
0
# Variable minimum value for gnuplot plots:
6
# Variable maximum value for gnuplot plots:
40
# Title string for salinity 3D NetCDF file:
'Diva 3D analysis of the variable'
# Variable long name string:
'Potential salinity'
# Variable units string:
'psu'
```

Example file 12.2: `3Dinfo` file

12.3 3D analyses: inputs preparation

The working directory for running a 3D Diva analysis is `DIVA3D/divastripped/` directory. All Diva 3D runs can be done by simply running the shell script `diva3Ddress`. The `diva3Ddress` performs the actions prescribed in the info file `3Dinfo`.

12.3.1 Coast contour files generation

To generate coast contour files for all the levels of which depth is present in the `contour.depth` file in the `divastripped/input`, one has to choose the flag number 1 or 3 in the `3Dinfo` file and provide as input in `divastripped/input` a bathymetry file of the area of interest. the input bathymetry file may be an ascii `topo.dat` or a GHER format binary file `topo.grd` and the related `TopoInfo.dat` as described in Section 7.2.2. A `param.par` file is also needed, and can be placed in the `divastripped/input` input directory.

The resulting coast contour files (coast.cont.1*xxxx*) are placed in the subdirectory input/divaparam/. If the chosen flag number for contour generation in the 3Dinfo file is 3, advection constraint files (anisotropic correlations along topography) are generated as well, and placed in input/divaUVcons subdirectory.

Input	Output
param.par, contour.depth topo.dat or topo.grd and TopoInfo.dat	coast.cont.1*xxxx* in divaparam Uvel.1*xxxx* and Vvel.1*xxxx* in divaUVcons

12.3.2 Data sets cleaning

All data sets provided in DIVA3D/divastripped/input/divadata/ can be cleaned from data points located outside the mesh and from suspected outliers. Choose a flag number corresponding to the desired action for data sets cleaning in the 3Dinfo file. A param.par file is also needed, and can be placed in the divastripped/input/ input directory.

At this stage, field of scaling factors to the correlation length can be generated on the basis of data distribution, and for the levels corresponding to each data set (see Section 12.2.2).

Input	Output in input/divadata/
param.par & var.1*xxxx*	var.1*xxxx*.notcln: original data set files var.1*xxxx*.clean: data set files cleaned from data out of the mesh var.1*xxxx*.withoutliers: data set files cleaned with outliers var.1*xxxx*: The cleaned data set files

12.3.3 Parameters optimisation

The estimation of analysis parameters (see Chapter 3) can be done for all levels using diva3Ddress. It is possible to optimise one or more parameter for a range of levels with different options (see Section 12.2.2). The parameters which can be optimised are correlation length L, signal-to-noise ratio λ and the error variance background $VARBAK$. The parameters optimisation can be done within a range of bounds (a maximum and a minimum). The bounds can be prescribed for all levels in the 3Dfile (see Section 12.2.2) or varying with levels by giving the list of bound in files CLminmax and/or SNminmax.

To perform parameters optimisation, one can place a default param.par with an approximated values for correlation length (L), signal-to-noise ratio (snr) and variance ($VARBAK$) parameter values, in input/divaparam/ (or input) directory). If parameter bounds are desired for each considered level, one can place a bound file corresponding to the parameter(s) to be optimised (CLminmax and/or SNminmax) in input/divaparam/, or prescribe a general one in 3Dinfo file. Choose the appropriate flag value in the 3Dinfo file (see Section 12.2.2). The 3D analysis parameter optimisation output is a set of param.par indexed following the variable name and the corresponding level, and summary files of estimated parameters before and/or after vertical filtering.

Input	Output in input/divaparam/
param.par in divaparam or in input/divaparam/	param.par.var.1*xxxx* with optimised L, snr, and $VARBAK$ var.CL.dat.filtered, var.CL.dat.notfiltered var.SN.dat.filtered, var.SN.dat.notfiltered var.VAR.dat.filtered, var.VAR.dat.notfiltered

12.4 Performing 3D analyses: diva3Ddress

12.4.1 A simple analysis: input files

Input files in divastripped/input/

The minimum input files for performing a Diva 3D analysis consists of:

- 3Dinfo file (see 12.2),
- contour.depth file (see 12.1),
- coast.cont.1*xxxx* files for all considered levels in divaparam subdirectory (see 12.3.1),
- param.par files:
  * param.par.var.1*xxxx* for all considered levels and prepared for the considered variable put in divaparam subdirectory, or
  * param.par.1*xxxx* for all considered levels divaparam subdirectory, or
  * one param.par file put in divastripped/input/ directory or in divastripped/input/divaparam/ subdirectory.
- data sets for all considered levels var.1*xxxx* files in divadata subdirectory.

Tips 12.2 *If for a level (or all levels) param.par.var.1xxxx is not present, one default param.par file must be placed in the divaparam subdirectory or in the input directory.* ■

Using relative length files:

If more than one relative length files are available, they must be named and numbered following the variable and level to which they correspond as RL.var.1*xxxx*, and must be provided in the input/divaparam/ subdirectory. One default file RL.dat may be placed in input/divaparam subdirectory to be used for the levels for which relative length files are missing. One RLinfo.dat ascii file (grid info file) must be placed with the relative length files (binary GHER format).

If only one RL.dat file of relative length is used, it must be placed in the divaparam subdirectory or in the input directory.

How to create these relative length files ?

If you do not have these binary relative length files, you can either create them by yourself or use the tool divaasctobin located in JRA4/Climatology which use simple ascii files as input to create your binary ones, via a run of diva. You will need to edit this script and set the parameter "RL" to 1 (at the beginning). Please note that this is not only a format transformation, the output is the analyse of the input files (with low SNR, high CL and reference field equal to one. By default, the domain (lon, lat, x and y step) is the one defined in the original ./input/param.par file.

Your ascii input files have to be located in JRA4/Climatology/input/divaparam. Your input files have to be named like this : ./input/divaparam/RL.var.1$xxxx$.ascii. They contain 3 columns : longitude, latitude and the value of the relative length.

Then, just launch ./divaasctobin in the directory JRA4/Climatology. The ouput binary files as well as the RLinfo.dat_erasethispart (of course, rename it by erasing the last part when activation is needed) will be located in input/divaparam, ready to be used. Do not forget to check if the output corresponds to what you want by looking at RL.10001000.4Danl.nc in output/3Danalysis.

> **Convention:** When a RLinfo.dat file is present in the divaparam subdirectory or in the input directory, Diva will perform 3D analysis using relative length files.

Using advection constraint

To perform 3D analysis with avection constraint, the files UVinfo.var.1$xxxx$, Uvel.var.1$xxxx$, Vvel.var.1$xxxx$, must be then placed in input/divaUVcons/ subdirectory. The advection constraint is activated when a constraint.dat file is present in the input directory (see Section 8.4). If one wants to use different advection parameters θ and $\mathcal{A}$ (see Section 8.5) a two column 3Dconstraint file must be placed in input/divaparam subdirectory where each line contains the advection parameters for the corresponding level number.

If UVinfo files are identical for all the levels, only one file UVinfo.dat may be placed in the input directory or in the input/divaUVcons subdirectory.

If for some levels, the pair of files Uvel.var.1$xxxx$, Vvel.var.1$xxxx$ (or Uvel.1$xxxx$, Vvel.1$xxxx$) is not available, A default Uvel.dat and Vvel.dat files must be placed in the input/divaUVcons/ subdirectory as well as a UVinfo.dat if using different UVinfo files.

If for all levels, the same advection files are used, only Uvel.dat, Vvel.dat and UVinfo.dat may be placed in the input/divaUVcons/ subdirectory or simply in the input directory.

How to create these advection files ?

If you do not have these binary advection files, you can either create them by yourself or use the tool divaasctobin located in JRA4/Climatology which use simple ascii files as input to create your binary ones, via a run of diva. You will need to edit this script

and set the parameter "UV" to 1 (at the beginning). Please note that this is not only a format transformation, the output is the analyse of the input files (with low SNR, high CL and reference field equal to zero. By default, the domain (lon, lat, x and y step) is the one defined in the original `./input/param.par` file.

Your ascii input files have to be located in `JRA4/Climatology/input/divaUVcons`. Your input files have to be named like this : `./input/divaUVcons/Uvel.1`$xxxx$`.ascii` and `./input/divaUVcons/Vvel.1`$xxxx$`.ascii`. They contain 3 columns : longitude, latitude and the value of the speed component.

Then, just launch `./divaasctobin` in the directory `JRA4/Climatology`. The ouput binary files as well as the `UVinfo.dat` will be located in `input/divaUVcons`, ready to be used. Do not forget to check if the output corresponds to what you want by looking at `Uvel.10001000.4Danl.nc` and `Vvel.10001000.4Danl.nc` in `output/3Danalysis`.

> **Convention:** The advection constraint is activated when a `3Dconstraint` file is present in the `divaparam` subdirectory or a `constraint.dat` is present in the `input` directory.

Using reference fields

If reference fields are present in the `input/divarefe` subdirectory, they will be used automatically by Diva to perform 3D analysis using the reference field files as a background.

To use a variable reference field as background for given level number, the `GridInfo.dat` and at least one of the three types of reference files `var.1`$xxxx$`.ascii.ref` (2D ascii file),`var.1`$xxxx$`.datapoint.ref` reference at data points or `var.1`$xxxx$`.ref` binary 2D GHER format must be present in the `divarefe` subdirectory.

> **Convention:** The use of reference fields for a given level is activated when the corresponding reference field files are present in the `divarefe` subdirectory.

Using detrending

To perform Diva 3D analysis with detrending of data, a `detrendinfo` file must be provided in the directory `input`. The `detrendinfo` has two columns and one line: where the group number of detrending is prescribed in the first column, and the iterations number in the second (see Section 5.3). In this case all data set files should have the right number of columns starting from the fifth and where classes are numbered.

> **Convention:** Diva 3D analysis with data detrending is activated when `detrendinfo` file is present in the `input` directory.

Running diva3Ddress

To run Diva to perform a 3D analysis, one has simply to run the shell script file diva3Ddress in divastripped. Diva 3D analysis outputs are normal analysis of a variable or reference fields, depending on the chosen flag number for analysis in the 3Dinfo (see Section 12.2.2).

12.4.2 Diva 3D analysis outputs

The outputs are placed in output/3Danalysis/ and consist of:

The 3D analysis files: in NetCDF and GHER binary format.

	var.1*xxxx*.1*yyyy*.fieldgher.anl
var.1*xxxx*.1*yyyy*.anl.nc	var.1*xxxx*.1*yyyy*.fieldgher.ref
var.1*xxxx*.1*yyyy*.errorfieldgher.anl	var.1*xxxx*.1*yyyy*.ref.nc

Figure 12.1: Content of output/3Danalysis/

The 3D variable analysis NetCDF file contains the diva analysis of the variable and a set of variable related information fields: relative error and error standard deviation fields, variable masked (using two relative error thresholds) fields, deepest values of the variable field and the related masked fields. It contains also fields of information about data distribution and outliers as well as fields of correlation length and signal-to-noise ratio parameters.

A subdirectory Fields containing all the Diva 2D output files for all levels:

GridInfo.dat	var.1*xxxx*.ref	var.1*xxxx*.error
var.1*xxxx*.anl	var.1*xxxx*.ascii.ref	var.1*xxxx*.errorascii
var.1*xxxx*.anl.nc	var.1*xxxx*.datapoint.ref	var.1*xxxx*.valatxyasc.ref
var.1*xxxx*.ascii.anl	var.1*xxxx*.ref.nc	valatxy.var.1*xxxx*
var.1*xxxx*.outliersbis	var.1*xxxx*.outliersbis.norm	

Figure 12.2: Content of output/3Danalysis/Fields/

A subdirectory datadetrend: it contains trend data set files for all levels trends.*i*.dat.var.1*xxxx* (*i* is the group number).

A subdirectory Meshes: it contains the mesh files, so that they can be re-used for other applications.

Log files Two log files are generated:

- diva.log: Log file of Fortran binaries run in ./output/
- var.diva3D.log: Log file of shell scripts execution in output/3Danalysis/.

13 Climatology production: Diva 4D

Diva can be used to produce climatologies for a given variable in an oceanic basin. In this case Diva 3D tools are used to produce for successive climatological time periods, 3D climatological analyses on the basin. The resulting climatologies are gathered in 4D binary files GHER format and NetCDF.

The working directory to performs 4D-analyses is:
`diva-x.x.x/JRA4/Climatology`.

Contents

13.1 Climatology definition

The climatologies to be produced are first defined by the mean of three files:

`varlist`:	one column file, where each line defines the short name of a variable (see example 13.1).
`yearlist`:	one column file, where the lines define the time period of years over which the climatologies (of the variables) are performed (see example 13.2).
`monthlist`:	one column file, where the lines define the time period in the year for which the climatologies (of the variables) are performed (see example 13.3).

```
Temperature
Salinity
```

Example file 13.1: `varlist`

```
19001950
19501980
19802012
```

Example file 13.2: yearlist

```
0103
0406
0709
1012
```

Example file 13.3: monthlist

Convention:

- In yearlist, each time period must be in an eight digits number such as *yyyyzzzz* where *yyyy* is the start year and *zzzz* the end year time period.
- In monthlist, each time period must be in a four digits number such as *mmnn* where *mm* is the start month and *nn* the last month numbers.
- In monthlist, if the first month is greater than the second (ex. 1202), the previous year is considered for months before January (ex. 12).

13.2 Diva 4D climatology performance

All Diva shell scripts files for climatologies (or 4D-analyses) production are located in diva-x.x.x/JRAx/Climatology. This directory has its proper subdirectories:

input where input data and files are placed and

output where Diva outputs are stored.

The main shell script file for generating climatologies is divadoall. The actions that performed when running divadoall are:

- Preparation of data files (ODV files without any depth axis and/or containing current -speed and direction- variables). Divadoall calls divanodepthODV4, generating new files with the extension "_bis.txt" containing the x and y components of the speed (u_star and v_star), as well as a depth axis.
- Data extraction at selected depth levels.
- Weighting of data. In case of close measurements (space and time), the representativity errors can be mitigated via a weighting option. The closer the measurements are, the less is their weight in the analysis. The characteristic distances for the weighting are defined by the user in radiusweighting.par, see file 13.4. In case of

file absence, the correlation length (from `param.par`) divided by 10 (same units as data) is used for the characteristic length scale, while the characteristic time scale is fixed to 7 days. This option is particularly suited for time series.

- Cleaning of duplicates in the extracted data (`divadoall` calls `divaduplicatesODV4` if the analysis flag is not zero).
- Boundary lines/coastline generation (contour files).
- Advection field generation based on coastlines.
- Cleaning of the data outside the mesh.
- Outliers elimination from data sets.
- Generation of relative length fields.
- Optimization of the correlation length (for each data set).
- Optimization of the signal-to-noise ratio (for each data set).
- Calculation of variable (semi-normed) reference fields.
- Performance of variable analysis fields using the following options:
  - analysis without option (normal variational analysis),
  - analysis using a reference fields,
  - analysis using advection constraint,
  - analysis with data transformation,
  - analysis using reference fields for each level calculated on bases of mixed data from three neighbouring levels,
  - analysis using a filtered mean background field: all levels mean are first calculated an vertically filtered before being used 3D analyses.
- Gnuplot plot production.
- Analysis with detrending method.

> **Note:**
> All actions performed by `divadoall` are prescribed in the file `driver` through flag values (see section 13.4.4 and example 13.5).

Note:

* When data extraction is activated in the `driver`, the execution is made for all levels found in `contour.depth` file provided in the subdirectory `input`. It is also taking into account a minimum number of data in a layer with regard to the corresponding flag value given in `driver`.
* When boundary line and coastline generation is activated in the `driver`, the execution is made for all levels found in `contour.depth` file provided in the subdirectory `input`.

* When parameter optimisation and/or analysis is activated, the execution is made for the levels between the values chosen for the lower and upper level numbers and takes into account the bound values (maximum and minimum) prescribed in `driver`. Be consistent between the values specified as lower/upper level and the depth levels listed in contour.depth (i.e., avoid to specify more levels than those listed in contour.depth).

All actions performed by `divadoall` use the input files:

`varlist`
`yearlist`
`monthlist`
	in `climatology` directory

`contour.depth`	in `climatology/input` directory
`param.par`	in `climatology/input` or in `climatology/input/divaparam` directory

13.3 Input data preparation

13.3.1 Data files

General Format

They **must** be ODV SeaDataNet compliant: https://www.bodc.ac.uk/data/codes_and_formats/odv_format/

- **Date column** : it is advised to use the most complete date format "yyyy-mm-ddThh:mm:ss.sss", or at least "yyyy-mm-ddT".
- **Detection of profiles** : the ODV profiles should always allow a combination "edmo code - local cdi" unique for each profile, and if these columns are absent (e.g. non-SDN profiles), DIVA uses a combination of "cruise", "station", "longitude" and "latitude". In a single profile, the time has to be constant, otherwise you will get a warning and your profile will be split.

Profiles and time series

Profiles and time series have to be in separated ODV files.

Missing value

In the comment lines, you can specify the input missing value as follows (not necessarily the same as the output exclusion value defined in `param.par`) :

```
//<MissingValueIndicators>NaN</MissingValueIndicators>
```

where "NaN" is the missing value.

13.3.2 Inputs for input data preparation actions

In Diva 4D (or Climatology production) we can use all the tools provided in Diva 3D for input data preparation. Input data preparation consists in the following actions:

- Data set for extraction.
- Weighting of extracted data.
- Boundary lines and coastlines generation and advection field generation.
- Data cleaning on mesh, outliers elimination from data sets and generation of Relative Length fields.
- Parameters optimisation and reference fields generation.

To perform an action, one has to configure the `driver` file and give in the corresponding flag values (see Section 13.4.4) and run the `godiva` file script (this will launch the `divadoall` script and check for possible severe errors). The standard output (stdout) and error (sdterr) will be stored in `divadoall.log` while the error and warning lines will be found in `divadoall.`
`severeerrors`, `divadoall.errors` and `divadoall.warnings`. For each action, specific inputs are needed:

Action	Inputs
Data extraction	`datasource` in `Climatology` `qflist` in `Climatology`

Data extraction **and** weighting	`datasource` in `Climatology`
	`qflist` in `Climatology`
	`radiusweighting.par` in `Climatology/input`

Coastline generation and "Advection" fields generation	`topogebco.asc`, `topo.gebco` or `topo.dat` ascii file or `topo.grd` GHER binary format file and its related `TopoInfo.dat` ascii info-file
Data cleaning on mesh, outliers elimination and generation of relative length fields	`divadata` a directory which contains data set files of the considered layers, `divaparam` a directory which contains coastlines `coast.cont.`$100xx$ files for all considered layers and a `param.par` file in `input` or `input/divaparam` directory
Parameters optimisation (L and S/N)	`divadata` directory which contains the data set files of the considered depths `divaparam` directory which contains coastlines `coast.cont.`$100xx$ files of the considered basin, and a(template) `param.par` file in `input` or `input/divaparam` directory.
Reference fields generation	`divadata` directory which contains the data set files of the considered depths and time periods `divaparam` directory which contains coastlines `coast.cont.`$100xx$ files of the considered basin, and a(template) `param.par` file in `input` or a `param.par.var.`$100xx$ files in `input/divaparam` directory. In these `param.par` and/or `param.`$100xx$ files, ireg is automatically forced to 0.

```
# characteristic length of weighting (same units as data) [not too low, otherwise memory problems can occur]
0.01
# characteristic time of weighting (days)
2
```

Example file 13.4: The `radiusweighting.par` file.

13.3.3 Outputs of input data preparation actions

Outputs resulting from a `divadoall` run for input data preparation actions are placed in the `input` directory for data sets extraction and in a `newinput` subdirectory for the other actions as shown in the following table:

Action	Outputs
Data extraction	A subdirectory `divadata` is created in `input` directory, and contains all the data sets.
Data weighting	The extracted data files in `input/divadata` contain a variable weight for each measurement.
Coastlines generation and "Advection" field generation	A `newinput` subdirectory which contains: a subdirectory `divaparam` with the `coast.cont.`$100xx$ and a subdirectory `divaUVcons_all` containing the velocity field files. All these files are also copied to subdirectories of `input`.
Data cleaning on mesh, outliers elimination and generation of relative length fields	A `newinput/divaparam` subdirectory which contains cleaned data sets and relative length files if generated.
Parameters optimisation (L and S/N)	A `newinput/divaparam` subdirectory which contains `param.par.var.`$100xx$ files and summary files of the optimisation and filtering procedure.
Reference fields generation	A `newinput/divarefe` subdirectory which contains all generated reference fields

The shell script file `divadocommit`: in order to be able to use the outputs of input data preparation actions, they must be copied to the `input` directory. This can be done by running the sell script file `divadocommit`.

Note:

divadocommit replaces input files in input directory by the ones found in newinput directory assuming that the driver, varlist, yearlist and monthlist files are the ones used by divadoall to create the newinput subdirectory on which divadocommit is run.

* When reference fields are generated, they are copied by the script file divadocommit in a subdirectory input/divarefe_all.

```
extract flag: 1 do it, 0 do nothing, -1 press coord, -10 pressure+Saunders
1
boundary lines and coastlines generation: 0 nothing, 1: contours, 2: UV, 3: 1+2
1
cleaning data on mesh: 1, 2: RL, 3: both, 4: 1 + outliers elimination, 5: =4+2
4
minimal number of data in a layer. If less, uses data from any month
10
isoptimise 0 nothing, 1 L, 2 SN, 3 both,  negative values filter vertically
0
Minimal L
0.1
Maximal L
1
Minimal SN
0.05
Maximal SN
0.5
2 do reference, 1 do analysis and 0 do nothing
1
lowerlevel number
7
upperlevel number
11
4D netcdf climatology file
0
isplot 0 or 1
1
number of groups for data detrending, 0 if no detrending.
0
```

Example file 13.5: The driver file.

13.4 Production of climatologies

Diva 4D allows the production of climatologies based on simple Diva data analysis or based on Diva analysis using various options as in Diva 3D:

- relative length (RL) files,
- advection constraint,
- reference fields and detrending.

Note: These options are automatically activated when the appropriate input data are provided.

Diva 4D for climatology production offers more options to improve the analysis coherence:

- analysis using vertically filtered mean background
- analysis with data transformation: log(data)-exp(analysis), *Logit* and *anamorphosis transformations or a "user defined" transformation.*
- *analysis using a reference field for each layer generated on the basis of all data from the two neighbouring layers in addition to the layer data set.*

Note: These options are activated with a specific flag values in the `driver`.
Note: The *Logit* transformation is made to insure analysis values to be in a given range $[a, b]$. The range $[a, b]$ must be prescribed in a file `var.logitrange` (see example 13.6) and provided in `input/divadata`. If `var.logitrange` is note provided and the *Logit* transformation is acctivated, Diva will take the data minimum and maximum values as rage values.

```
 0
10
```

Example file 13.6: Example of file `var.logitrange`.

13.4.1 Inputs for production of climatologies

in `climatology` directory

`varlist`
`yearlist`
`monthlist`
	input files defining the climatology

`constandrefe`	input file to activate advection constraint and/or reference fields

in `climatology/input` directory

`contour.depth`	file of depth values (see example 12.1)
`param.par`	file defining the analysis parameters, provided here if not present in `divaparam`
`NCDFinfo`	Info file containing metadata for NetCDF files (see example 13.7)
`divaparam`	subdirectory containing coastline files `coast.cont.`$100xx$ and parameters files `param.par.var.`$100xx$
`divadata`	subdirectory containing data set files `var.yyyyzzzz.mmnn.`$100xx$
`divarefe_all`	subdirectory containing reference field files (see Section 12.4.1)
`divaUVcons_all`	subdirectory containing advection constraint fields (see Section 12.4.1)

```
 Title string for 3D NetCDF file:
'Diva 3D analysis '
 Reference time for data (if not climatological data)
'months since since xxxx-01-01'
 Time value (if not climatological data)
1200
 Cell_method string:
'time: mean (this month data from all years)'
 Institution name: where the dataset was produced.
'University of Liege, AGO, GHER'
 Production group and e-mail
'Diva group. E-mails : JM.Beckers@ulg.ac.be'
 Source (observation, radiosonde, database, model-generated data,...)
' data_from various sources'
Comment
'This is only for DIVA development and testing work'
Author e-mail address (or contact person to report problems)
'swatelet@ulg.ac.be'
```

Example file 13.7: NCDFinfo

13.4.2 Advection constraint and reference field files

To perform Diva 4D analyses with advection constraint and/or using reference fields, the advection constraint and reference field files must be provided in the corresponding subdirectory `divarefe_all` and `divaUVcon_all` in `input` directory (see Sections 12.4.1 and 12.4.1).

Note:

The naming conventions for advection field and advection constraint field files is the same as for Diva 3D: advection condtraint files are named as:
`UVinfo.var.yyyy.zzzz.mmnn.1`$xxxx$,
`Uvel.var.yyyy.zzzz.mmnn.1`$xxxx$,
`Vvel.var.yyyy.zzzz.mmnn.1`$xxxx$, and a `constraint.dat` file,
and for reference fild files:
`var.yyyy.zzzz.mmnn.1`$xxxx$`.ascii.ref`,
`var.yyyy.zzzz.mmnn.1`$xxxx$`.datapoint.ref` and
`var.yyyyzzzz.mmnn.1`$xxxx$`.ref`

Using advection constraint and/or reference field

The advection constraint and/or reference fields usage actions are activated by the corresponding flag values in `constandrefe` file.The advection constraint option is activated when the corresponding flag value is equal to 1. The use of reference fields option is activated when the corresponding flag value is equal to 1, in this case a year period and month period codes must be provided in the corresponding lines.

```
# advection flag
0
# reference field flag
1
# variable year code
19002010
# variable month code
0103
```

Example file 13.8: constandrefe

How to use a different reference field for each month period ?

Just change the parameter "refsameasmonthlist" to "yes" in the script `divadoall` (around line 330). The month code for your reference field will then be the same as the current month period. Do not forget to set "refsameasmonthlist" back to "no" after your analyses.

13.4.3 Diva 4D climatology production output

The outputs are placed in `output/3Danalysis/` and are the same as of the Diva 3D, in addition to the climatologies 4D-NetCDF files:

The 4D analysis files: in NetCDF and GHER binary format.

`var.`*yyyyzzzz*`.4Danl.nc` or `var.4Danl.nc` (of all year periods)

The 4D variable analysis NetCDF file contains the diva analysis of the variable and a set of variable related information fields: relative error and error standard deviation fields, variable masked (using two relative error thresholds) fields, deepest values of the variable field and the related masked fields. It contains also fields of information about data distribution and outliers as well as fields of correlation length and signal-to-noise ratio parameters.

The 3D analysis files: in NetCDF and GHER binary format.

`var.`*yyyyzzzz.mmnn*`.1`*xxxx*`.1`*yyyy*`.anl.nc`
`var.`*yyyyzzzz.mmnn*`.1`*xxxx*`.1`*yyyy*`.errorfieldgher.anl`
`var.`*yyyyzzzz.mmnn*`.1`*xxxx*`.1`*yyyy*`.fieldgher.anl`
`var.`*yyyyzzzz.mmnn*`.1`*xxxx*`.1`*yyyy*`.fieldgher.ref`
`var.`*yyyyzzzz.mmnn*`.1`*xxxx*`.1`*yyyy*`.ref.nc`

A subdirectory `Fields` containing all the Diva 2D output files for all levels:

`GridInfo.dat`	`var.`*yyyyzzzz.mmnn*`.1`*xxxx*`.ref`
`var.`*yyyyzzzz.mmnn*`.1`*xxxx*`.anl`	`var.`*yyyyzzzz.mmnn*`.1`*xxxx*`.ascii.ref`
`var.`*yyyyzzzz.mmnn*`.1`*xxxx*`.anl.nc`	`var.`*yyyyzzzz.mmnn*`.1`*xxxx*`.datapoint.ref`
`var.`*yyyyzzzz.mmnn*`.1`*xxxx*`.ascii.anl`	`var.`*yyyyzzzz.mmnn*`.1`*xxxx*`.ref.nc`
`var.`*yyyyzzzz.mmnn*`.1`*xxxx*`.outliersbis`	`var.`*yyyyzzzz.mmnn*`.1`*xxxx*`.outliersbis.norm`
`var.`*yyyyzzzz.mmnn*`.1`*xxxx*`.error`	
`var.`*yyyyzzzz.mmnn*`.1`*xxxx*`.errorascii`	
`var.`*yyyyzzzz.mmnn*`.1`*xxxx*`.valatxyasc.ref`	
`valatxy.var.`*yyyyzzzz.mmnn*`.1`*xxxx*	

A subdirectory `datadetrend`: it contains trend data set files for all levels `trends.`*i*`.dat.var.`*yyyyzzzz.mmnn*`.1`*xxxx* (*i* is the group number).

A subdirectory `Meshes`: it contains the mesh files, so that they can be re-used for other applications.

Log and metadata files: Two log files and a text metadata file are generated:

- `var.Metainfo.txt`: All the information about domain, grid, variable, and run parameters.
- `var.`*yyyyzzzz.mmnn*`.Fortran.log`: Log file of fortran binaries run.
- `var.`*yyyyzzzz.mmnn*`.diva3D.log`: Log file of shell scripts execution.

13.4.4 `driver` file: actions and flag values

All actions performed by `divadoall` are prescribed in the file `driver` through flag values. In this section all possible actions and corresponding flag values are listed:

- **Data extraction**: Possible flag values: 0,1,2,3,−1 and −10. If you activate the data extraction (flag value $\neq 0$) in the `driver` file, the execution of `divadoall` will run the `divaselectorODV4` automatically, including interpolation to the levels specified in `contour.depth`. Data will be extracted from the ODV spreadsheat file(s) specified in `datasource`. Command `divaselectorODV4` will recognises if the data export to ODV file was done with depths (in meters) or it was done with pressure (in dbar) vertical coordinate, you can either choose to map it as if they were meters or apply the Saunders (1981) correction. Choose flag = −1 to use pressure coordinate and assume they are meters, and flag value = −10 to use pressure coordinates and transform to meters by using the Saunders approach.

  If you choose the flag = 2, the weighting option will be activated. Particularly suited for time series or in other cases of overabundant data in some limited spatial and temporal zones.

  If you choose the flag = 3, the extraction will be performed from the bottom.

  If there is a `qflist` file, the selection with `divaselectorODV4` will only use those measurements for which the quality flag is one of those found in the file `qflist`. In the absence of `qflist` (or if `qflist` is empty), no quality flag analysis is done and all data taken.

  Note: you can specify several ODV4 spreadsheet files as input files, one file name (or full path) per line in `datasource` file, *they must have the same variables naming convention*. You can also specify different quality flags for each file by adding these values after the file name (separated by a space). At the moment, a maximum of two quality flags per file is admitted. In the absence of quality flag after the file name, `Diva` simply uses the values provided in `qflist`.

  Note: the files without any depth axis are treated separately by `divanodepthODV4`. The minimum and maximum instrument depth (metadata) are used to recreate an artificial depth axis which can be used by diva. Please note that, in this case, each file without depth axis (in datasource) should contain only one location (otherwise, the other ones are not used). This script also handles the current direction (CurrDir [deg T]) and speed (CurrSpd [cm/s]) and transforms them into x-y components (North, East). In this second case, depth axis has to be present. In any case, `divanodepthODV4` can only deal with a maximum of 2 scalar variables (+ current direction and speed). If you need to analyse more than 2 scalar variables, you can proceed by steps (just changing the `varlist`).

- **Boundary lines and coastlines generation**: Possible flag values are 0, 1, 2, 3 and 4. When this action is activated (flag ≥ 1), you must provide in the `input` directory the files `TopoInfo.dat` and `topo.grd` in addition to `contour.depth` file.

  * = 1 if contour files are to be generated,
  * = 2 if advection constraint (Anisotropic correlation along topography) files are to be generated from `topo.grd`,

  * = 3 if contour files and advection constraint are to be generated,
  * = 4 if advection constraint (Anisotropic correlation along topography) files are to be generated from `topo.grd`, in coherence with the relative length field generated when the cleaning index is set to 7.

- **Cleaning data and Relative Length**: Possible flag values are 0, 1, 2, 3, 4, 5, 6 and 7:
  * = 1 if data files are to be cleaned,
  * = 2 if relative length files depending on data coverage are to be generated,
  * = 3 if data files are to be cleaned and relative length files depending on data coverage are to be generated.
  * = 4 if outliers are to be cleaned from data files.
  * = 5 if outliers are to be cleaned from data files and, relative length files depending on data coverage to be generated.
  * = 6 if data files are to be cleaned and relative length files depending on depth to be generated.
  * = 7 if data files are to be cleaned and relative length files depending on the gradient of depth to be generated.
- **Minimum number of data in a layer**: Any value from -1 to infinity. If less, uses data from any month.
  * = -1 if you never want to use other data from other months.
- **Parameter optimization**: Possible flag values are 0, 1, 2, 3, -1, -2, -3, 10, -10, 30 and -30:
  * = 1 if correlation length parameters are to be estimated,
  * = 2 if signal-to-noise ratio (S/N) parameters are to be estimated,
  * = -1 if correlation length parameters are to be estimated and vertically filtered,
  * = -2 if signal-to-noise ratio (S/N) parameters are to be estimated and vertically filtered,
  * = 3 if both correlation length and signal-to-noise ratio parameters are to be estimated,
  * = -3 if both correlation length and signal-to-noise ratio parameters are to be estimated and vertically filtered,
  * = 10 if correlation length parameters are to be estimated using data mean distance as a minimum,
  * = -10 if correlation length parameters are to be estimated using data mean distance as a minimum and vertically filtered,
  * = 30 if both correlation length and signal-to-noise ratio parameters are to be estimated using data mean distance as a minimum (for L),

  * = −30 if both correlation length and signal-to-noise ratio parameters are to be estimated using data mean distance as a minimum (for L), and both parameters vertically filtered.

- **Analysis**: analysis and reference fields can be performed in different ways:
  - **Perform analysis**: Possible flag values are 1, 11, 12, 13 and 14:
    * = 1 if analysis fields of the given variable are to be performed for all the layers between L_1 and L_2 which are the flag values for lower level number and upper level number in the `driver`.
    * = 11 if analysis fields of the given variable are to be performed with log(data)-exp(analysis) transformation
    * = 12 if analysis fields of the given variable are to be performed with *Logit* transformation
    * = 13 if analysis fields of the given variable are to be performed with *anamorphosis transformation*
    * = 14 *if analysis fields of the given variable are to be performed with user chosen transformation function.*
  - **Perform reference fields**: Possible flag values are 2, 21, 22, 23 and 24:
    * = 2 if semi normed reference fields of the given variables (prescribed in `varlist` and for time periods described in `yearlist` and `monthlist`) are to be performed for all the layers between L_1 and L_2, which are the flag values for lower level number and upper level number in the `driver`.
    * = 21 if analysis fields of the given variable are to be performed with log(data)-exp(analysis) transformation
    * = 22 if analysis fields of the given variable are to be performed with *Logit* transformation
    * = 23 if reference fields of the given variable are to be performed with *anamorphosis transformation*
    * = 24 *if reference fields of the given variable are to be performed with user chosen transformation function.*
  - **Adding** 100 **to the flag value**:
    * = 101 or = $11x$ allows performing analysis using reference fields for each layer using all data from the two neighbouring layers in addition to the layer data set. Only reference fields are performed
    * = 102 or = $12x$ allows performing reference fields for each layer using all data from the two neighbouring layers in addition to the layer data set.

- **4D netcdf files generation**: Possible flag values are 0, 1 and 11:
  * = 0 or 1 If you only want 3D netcdf output files and a 4D netcdf for each year period,
  * = 11 If you also want a big 4D netcdf containing all the year period.

- **Gnuplot plots**: Possible flag values are 0 and 1. Activate this action for a quick visualization (and assessment) of the climatology production, `gnuplot` executions can be included in the production process.

  There are a few controls you can apply for these gnuplot plots:

* `VAR.bounds`: contains the lower and upper bounds during the plotting for the variable `VAR` (which is one of the variable names found in `varlist`), see example 13.9

```
# lower bound
0
# upper bound
30
```

Example file 13.9: `VAR.bounds`

* `VAR.pal`: contains the color palette for the same variable.
* `plotboundingbox.dat`: contains the box for plotting. This is typically used to plot only the region of interest, without overlapping regions with other climatologies (the numerical fields include the overlapping regions, only the plotting is limited with the `plotboundingbox.dat` file).

Note: the gnuplot colorbars use a scale that is actually remapped to the bounds found in `VAR.bounds`. Example: if your colorbar definition goes from 0 to 10 and the `VAR` bounds are from 0 and 100, a value of 50 in the variable analysed will use the color found in the colorbar definition at value 5. To help you designing a specially adapted color bar lets say for salinity, it is therefore a good idea to define the colorbar with the same bounds as those in `VAR.bounds`.

Note: for adapting the color palette, file `gnuplotcolornames` contains a list of pre-existing colors and their hexadecimal codes you can use instead of names.

- **Detrending** Possible flag values are 0 and n: the action is activated when choosing flag value an integer $n > 0$. The chosen value n must be equal or smaller to groups number in data files.

  Note: If you use `divadoall` (or `divaselectorODV4`) to extract data and create data input files, columns 5, 6 ,7 and 8 contain respectively groups years, months, days and hours (1 for the first year in the selection etc).

13.4.5 Producing bottom climatologies

Here are the steps to produce climatologies at a certain distance from the ocean bottom (unlike previous sections where the distance is counted from the surface).

1. Create a fine topography in GHER format, in files `topo_fine.grd` and `topoInfo_fine.dat`. The simplest option is to copy them from `topo.grd` and `topoInfo.dat`, while it is also possible to derive them by using the bathymetry provided by EMODnet. Once you have downloaded one of their NetCDF file, you can transform it to gher format by using the command `emobath2ghertopo`. Do not forget to first edit the script in order to specify the paths.

2. Specify the distances from the bottom in the file `contour.depth`. Important convention : the deepest layer is still on the first line, meaning you have to write the smallest distance from the bottom first. See example file 13.10.

3. Set the extraction index to 3 in the file `driver`.
4. Launch `divadoall`.
5. Launch `divadocommit`.
6. Optional: set the cleaning index to 7 in the file `driver`, in order to generate a relative length field depending on the gradient of the depth. This reduces the correlation length where the slope is too steep.
7. Optional: Launch `divadoall`.
8. Optional: Launch `divadocommit`. A file `theta.dat` is created in `input/divaparam` and contains the advised θ parameter for the use of the advection constraint in the analysis (last step).
9. Optional: set the coastlines index to 4 in the file `driver`, so that the generated velocity field is coherent with the relative length field previously generated, and increase the correlation length in directions where the bottom is flat. In this case, the new correlation length is equal to the correlation length provided by the user in `param.par`.
10. Launch `divadoall`.
11. Launch `divadocommit`.
12. Set the analysis index to 1 in the file `driver`.
13. Optional: use the θ from the file `theta.dat` to replace the first number of the file `constraint.dat`.
14. Optional: activate the advection constraint in the file `constandrefe`.
15. Launch `divadoall`.

```
0
50
100
```

Example file 13.10: `contour.depth`

Remark: during the extraction process (index = 3), the observations located between or close to the levels specified in `contour.depth` are interpolated vertically. But, if the observations are all below the levels specified, the closest (deeper) data will also be used, if it is not too far. The limit is 1000 m if $z >= 1300$ m, 400 m if $z >= 500$, 200 m otherwise.

13.5 Climatologies postprocessing

13.5.1 Cutting the 4D-NetCDF domain

1. Create a contour file in JRA4/Climatology/input such as `cutNCDF.cont`, see example file 13.11 for a square-shaped contour. First line : number of contours (has to be 1 for the moment), second line : number of points, other lines : lon and lat of the successive contour points.

2. Edit divacutNCDF : the first lines (USER SETTINGS) allow you to define the original 4D netcdf file (in `output/3Danalysis`), the contour file and the output 4D cut file.

3. Launch `divacutNCDF` in JRA4/Climatology.

```
1
4
33.00 40.00
33.00 48.00
45.00 48.00
45.00 40.00
```

Example file 13.11: `cutNCDF.cont`

Part IV

Appendix

A Problems...and solutions!

This chapter contains a list of Frequently Asked Questions concerning many aspects of Diva as well as a list of solved issues or bugs.

Contents

A.1 FAQ

A.1.1 Where can I find the latest version?

The latest stable version if available at http://modb.oce.ulg.ac.be/mediawiki/index.php/DIVA#How_to_get_the_code.3F.

A.1.2 What do I need to install DIVA?

Check Chapter 1 where the requirements and the procedure are described.

A.1.3 Is there a graphical user interface?

Previously, an interface for the 2-D version was available, but is was not up-to-date with respect to the developments of the code.

Usually, one wants to perform a large number (more than 100) analysis in order to produce a complete climatology. To this end, it is easier to use command line than to click and wait 100 times.

For the users not familiar with shells and scripts, the web interface (Barth *et al.*, 2010) can be tried at http://gher-diva.phys.ulg.ac.be/web-vis/diva.html

A.1.4 Can I use Diva to interpolate measurements from satellite?

Yes, it is always possible to perform an interpolation with Diva on this kind of data. However, a better solution is to take into account not only a single satellite images, but also the information contained in the images of the previous days. This is done with the software DINEOF (e.g., Alvera-Azcárate *et al.*, 2005; Beckers *et al.*, 2006, or http://modb.oce.ulg.ac.be/mediawiki/index.php/DINEOF).

A.1.5 How to report a bug or a problem?

The preferred options are:

1. to send a message to the Diva user group on google:
   http://groups.google.com/group/diva_users or
2. to open an issue on GitHub: https://github.com/gher-ulg/DIVA/issues

The advantage over emails is twofold: the questions is directly sent to all the Diva developers and the issues previously solved are archived and available for other users.

Along with a small description of the problem, add relevant informations that would help us solving your issue:

- the version of Diva you are using,
- your operating system (O. S.),
- your options for compiling the code
  (check file `compilation.log` in directory `DIVA3D/src/Fortran/`.

If the problem can be reproduced at the 2-D level (i.e., working in the directory `divastripped`), add the input files that generated the problem as well, so that we can check if the issue is machine-dependent.

To know your O.S. you can type in the shell:

```
gherulg$ uname -voi
28-Ubuntu SMP Tue Oct 9 19:31:23 UTC 2012 x86_64 GNU/Linux
```

If you received advice which helped you to solve the problem, please post a comment so that others know the solution worked or close the issue opened on GitHub.

A.1.6 How to register to the user group?

- Go to http://groups.google.com/group/diva_users and login with a google account (not necessarily a gmail address).
- Follow the "*Apply for membership*" link. You will be asked to explain why you want to use Diva.
- Finally click on the "*Apply to join this group*" button.
  You will get an email confirmation once the the application has been reviewed and accepted.

A.1.7 How can I use Diva in R, Matlab, IDL, Ferret or any other software

There are basically two ways:

a) Using special binaries and preparing `fort.*` files for Diva

This approach has been taken in the incorporation of Diva into ODV and in the Matlab function in http://modb.oce.ulg.ac.be/mediawiki/upload/divaformatlab.zip

It requires some time (you can try to understand the matlab function to see how to prepare the files and recover the results), but has the advantage that you do not need to install Diva, compilers, NetCDF or Cygwin. It also avoids creation of large subdirectory trees for Diva.

b) Using a full Diva installation and preparation of normal Diva input files

In this case you must have installed the Diva package and have access to either directly unix or Cygwin shells.

You also need to prepare a shell script that we will call `mydivacall` in this example, and which contains the instructions to be to executed with Diva. So typically what you would type in the command-line session when trying to make the analysis.

```
#!/bin/bash
export LC_ALL=C
PATH=$PATH:.
cd /home
pwd
echo This is a test
echo Hello Diva world
...
# Then go into the divastripped directory and run the scripts you want
```

Example file A.1: mydivacall

Then your program has to prepare all input files exactly as for a normal Diva execution. Once this is done, your program needs to make a system call (look at the documentation of your program on how to do it). On a Unix machine you would then simply include a command like

```
call system("/home/<path>/mydivacall")
```

For a Cygwin system it is more complicated:

```
call system("c:\cygwin\bin\bash.exe --login -i -c c:/<path>/mydivacall")
```

Once the script execution is finished, you can read the diva output files with your program and continue the processing.

A.1.8 What value for parameter `ireg` should I choose for a semi-normed analysis

The best option is to choose `ireg` = 0.

The command `divaseminorm` performs four operations:

1. divarefe = computing a reference fields with large value for L (your value multiplied by 5) and low signal-to-noise ratio (your value divided by 10)
2. divaanom: difference between your data values and the reference field at these data points
3. divacalc: performs a Diva analysis with the parameters you put in param.par, on the data anomaly. This is why you should choose ireg=0: you are working with anomalies, thus no need to subtract any background field.
4. divasumup: reconstruction of the analysed field by summing the reference and anomaly fields.

A.1.9 How can one create monthly analysis where the reference field is the annual analysis?

The latest version of divaanom is able to use an existing reference field. This field should be present as a binary file in the output directory with the name fieldgher.anl.ref, and the GridInfo.dat file should be present in output/ghertonetcdf/ directory.

An execution of divaanom will provide you with data.dat which contains anomalies with respect to your reference field (annual analysis in this case). Then you can work with data.dat as usual.

The last step is to apply divasumup to reconstruct the field by summing the anomaly analysis and the reference field.

In summary the steps to follow are:

1. apply divadress to the annual data (after the optimisation of the parameters),
2. copy the output fieldgher.anl with the name fieldgher.anl.ref,
3. for each month:
   (a) copy the corresponding data file into the input directory,
   (b) apply divaanom,
   (c) perform an analysis on the anomalies,
   (d) apply divasumup.

A.1.10 How to contribute to the development?

Any suggestion concerning the development of the software is welcome. Simply send to the developers or to the google group, a description of what improvements/tools you would like to see and we will check if this could be easily added to the general distribution.

A.1.11 How can I run Diva on a multi-processor machine?

Coarse grain parallelisation

The best option is to copy the whole directory `divastripped` in the directory in which it is located, but with a different name (e.g., `divastripped2`, or `divastripped_username1`). The you can run Diva analysis separately in these directories.

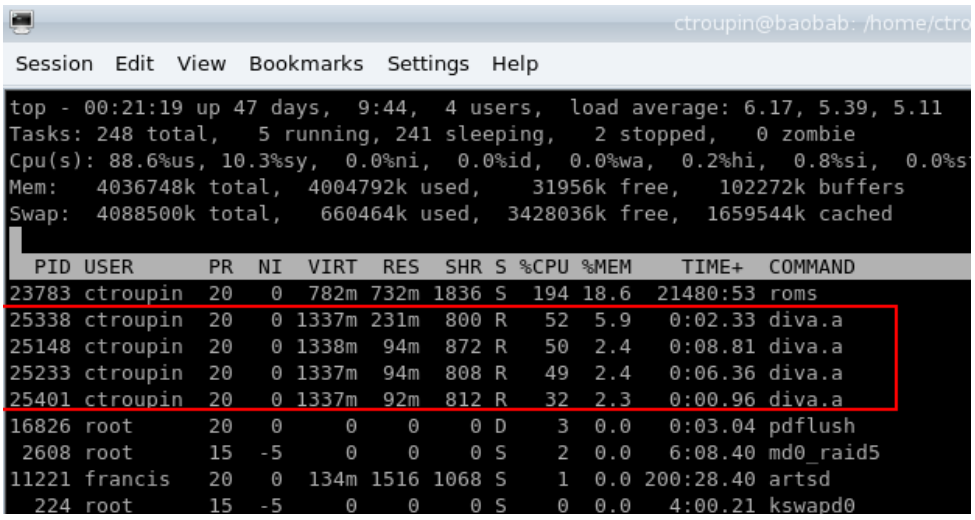


Figure A.1: Simultaneous run of Diva.

Fine grain parallelisation

If you compiled Diva for parallel use, you can activate the parallel solver by editing `divacalc` and use `solver=1`

A.1.12 What is the resolution of the output field?

One has to distinguish between 2 *resolutions*:

1. the resolution brought by the finite-element mesh, of which the characteristic length should be in agreement with the typical scale of the studied region (based on the data correlation in Diva);
2. the grid resolution, which can be anything (larger, smaller or similar to the mesh resolution). It means that you can always work with a finer grid, but that does not mean that the actual resolution will be improved.

So the best resolution you can obtain is the one allowed you by the data you are working with.

A.1.13 Why is there an iterative solver?

You can activate an iterative solver by editing `divacalc` and use `solver=2`. This can be useful if you do not calculate error fields and do not use cross validation techniques but work with very fine grids. In this case execution time can be reduced. There are some tuning parameters which can enhance convergence but to exploit them, please contact us.

A.1.14 Can Diva deal with several measurements at the same location?

Yes. In that case (for example: time series, mooring, ...) Diva provides an average value.

However, when data locations are very close and values are very different and a huge signal-to-noise ratio is used, then you will see artefacts simply showing that you have created a huge gradient because you said to Diva your data are perfect and yet are very different at very close stations. Figure A.2 provides an example of a situation with two different measurements at the same point.

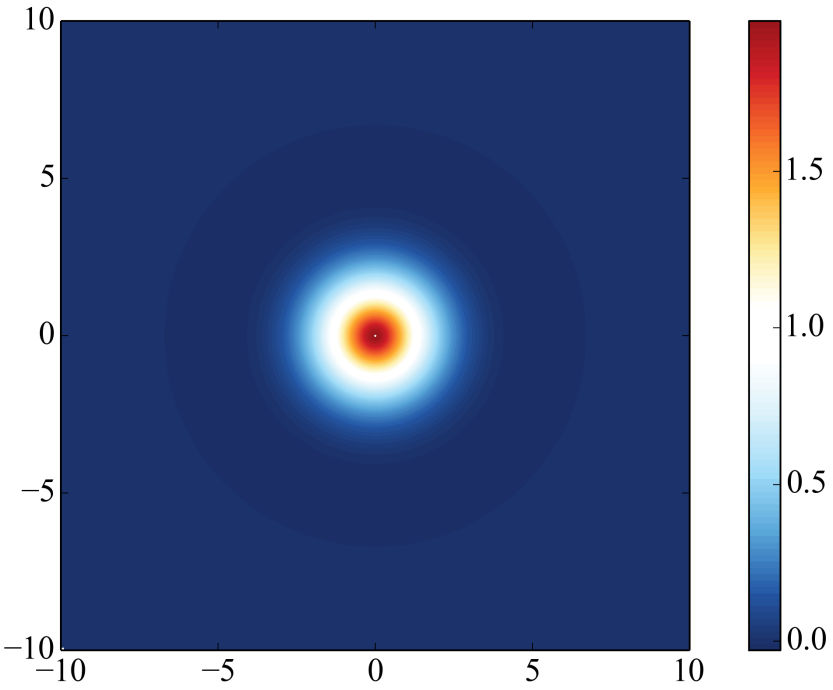


Figure A.2: Results with two data points with values 1 and 3, located in the domain center (0,0), with a large signal-to-noise ratio. The analyzed field at (0,0) is ≈ 2.

New : You can also activate the weighting option in the driver file (DIVA 4D) in order to give less importance to measurements very close (in space and time) to other ones. This option will limit the above artefacts. Further details in Section 13.2.

A.1.15 How to run Diva in operational or real-time mode?

The idea is to work on a data set that evolved regularly, let's say every day. It is assumed that the files are formatted so that they can be ingested by Diva (either ODV format for 4D runs, or simple 3-column files for 2D runs), and that a script `mydivarun` prepares the input files, execute Diva and copy the results into another directory.

On Unix-like computers, the software utility `cron` can be used to schedule a task, such as a Diva execution. Please consult the documentation relative to `cron` and `crontab`, for example: http://ss64.com/bash/crontab.html or http://cronjob.com/.

To have `mydivarun` executed every day at 9.15 AM, the crontab has to be edited:

```
gherulg$ crontab -e
```

and a line such as

```
gherulg$ 9 15 * * *   path_to_scripts/mydivarun
```

is added. If everything goes well, you can skip the rest of this section.

Otherwise, if the script runs properly when called directly from the shell, but not from the cronjob, it is probably due to the environment variables (PATH, LD_LIBRARY_PATH ...) passed by cron are minimal. For example your path used by cron is not the same path that you have when typing commands. To avoid this problem:

- Use absolute path for your commands. Note that Diva commands (`divacalc`, `divamesh`, ...) have to be run from the `DIVA3D/divastripped/` directory. Hence in the script `mydivarun`, you may write something like

  ```
  here=$pwd
  divadir=path_to_divadir
  cd $divadir
  ./divadress
  cd $here
  ```

- Manually add the path at the beginning of the script you want to run.

A good idea for debugging is to redirect the standard output and error in text files:

```
gherulg$ 9 15 * * *   path_to_scripts/mydivarun >
   path_to_directory/crontab.out 2>/home/ctroupin/DataOceano/
   AVISO/Operational/crontab.err
```

A list of possible reasons for cron job failure is found at
http://askubuntu.com/questions/23009/reasons-why-crontab-does-not-work.

A.1.16 How to run Diva on the Lemaitre2 cluster ?

1. Copy the whole DIVA directory to your scratch directory on the cluster (don't forget to regularly save the important files to your home directory).

2. Recompile the sources with `divacompileall`.
3. Install dos2unix and (if mandatory) gnuplot in a new directory `/bin` and add this directory to the $PATH.
4. Write a submission script to launch a new job (see this example : www.ceci-hpc.be/assets/doc/submission.sh).

More information can be found at http://www.ceci-hpc.be/

A.2 Error messages

A.2.1 "Command not found" message

```
MacBook-Pro-de-GHER:divastripped gherulg$ divatest
-bash: divatest: command not found
```

Why do I get this error?

Although you are in the correct directory, the command is not found. This is because the current directory (represented by `./`) is not in the path of your system.

How to solve it?

You can type
`./name_of_the_command`
so that the system knows the command is the current directory.

A better solution is to adapt your path by typing:
`PATH=$PATH:path_to_diva_directory`, where `path\_to\_diva\_directory` has to be adapted to your installation.

For example:

```
ctroupin@predator ~/Software/Diva/DIVA3D/divastripped $ pwd
/home/ctroupin/Software/Diva/DIVA3D/divastripped
ctroupin@predator ~/Software/Diva/DIVA3D/divastripped $export
   PATH=$PATH:home/ctroupin/Software/Diva/DIVA3D/divastripped
ctroupin@predator ~/Software/Diva/DIVA3D/divastripped $ echo $
   PATH
/usr/local/sbin:/usr/local/bin:/usr/sbin:/usr/bin:/home/
   ctroupin/Software/Diva/DIVA3D/divastripped/
```

For example in `cygwin`:

- go in the `/ect/`

- edit file `bash.bashrc` file and add the following line:
  export `PATH=$PATH:.`
- type `source bash.bashrc` in order to take into account the modification made.

A.2.2 Analysed field with white boxes near boundaries

The analysed fields has points of *not-a-number* (NaN) values.

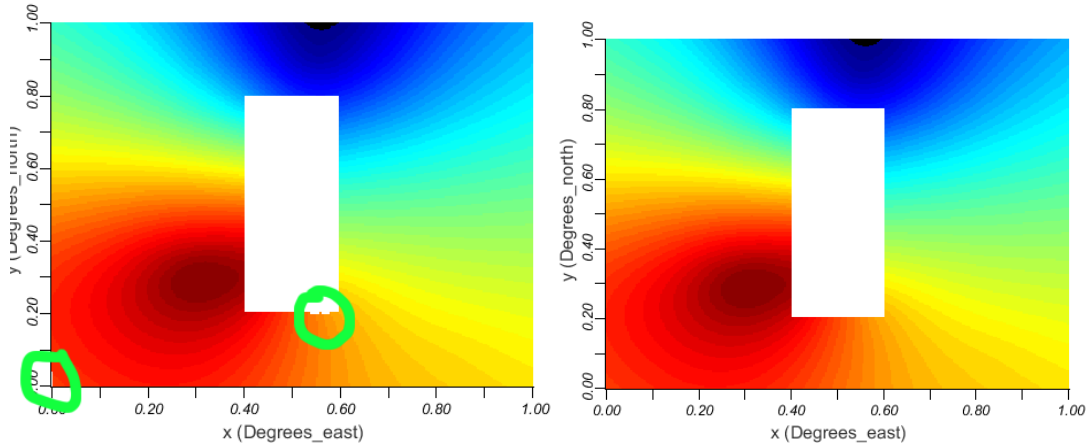


Figure A.3: Examples of Diva outputs with zones of NaN at boundaries. For the right the solution to the problem was applied

Why do I get this error?

This problem arises from the fact that you request the analysis almost exactly on the boundary.

How to solve it?

Internally Diva makes some coordinates changes and therefore roundings on boundary positions. The decision of a point falls in the domain or not can therefore be very sensitive to rounding if you place a request for analysis "exactly" on the boundary. In real situations, this very rarely happens, but when you use synthetic test cases, use contours and analysis points which do not coincide (look at `divatest` how the contour is made to avoid falling on the grid points of the analysis).

A.2.3 Command-line scripts not working

Why do I get this error?

End of lines in Unix, Windows and Mac files are different, and this causes problems when switching from a system to the other. Typically if you visualize a Windows-end-of-line file under Unix, you will see ends of line with symbols such as `^M` or `\r`. When reading

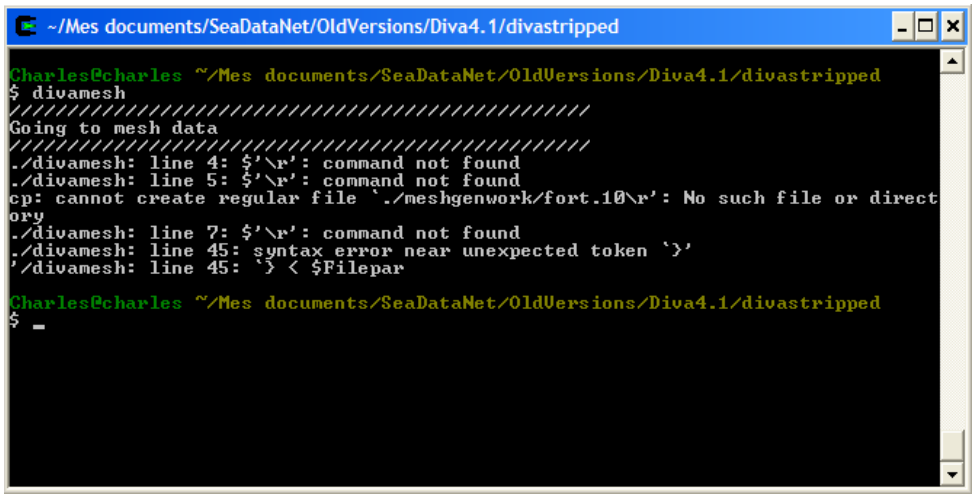


Figure A.4: Error messages due to bad ends of lines.

such files, scripts get in trouble because they expect to read numbers, but instead they find characters.

Note: strange behaviours of Diva are often related to this topic, therefore always be aware of this possible problem before undertaking more complex actions.

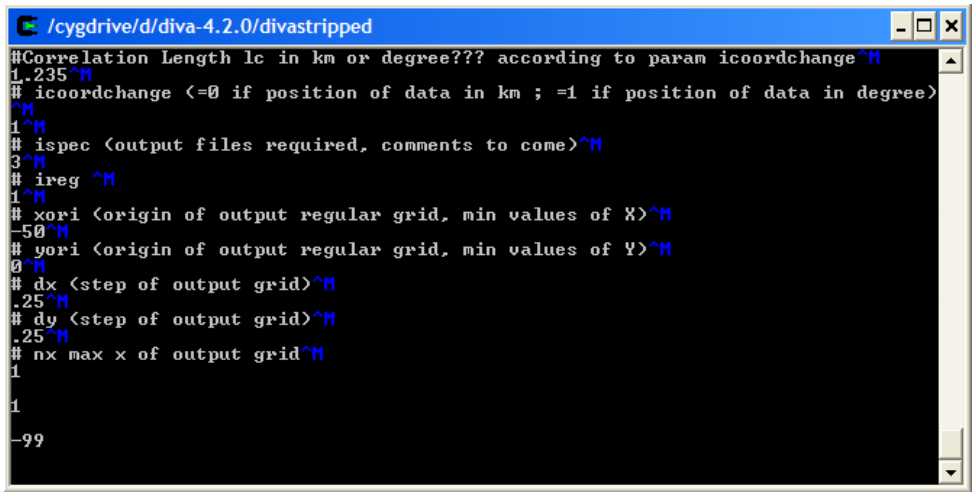


Figure A.5: Example of bad ends of lines.

How to solve it?

Working on a individual file, the command

```
[divastripped]$ dos2unix  file2convert
```

does the conversion between Windows and Unix end of lines. According to the Linux distribution, `dos2unix` may requires options to perform the conversion. For example with Mandriva 2010, it is necessary to add the option `-U`:

```
[divastripped]$ dos2unix  -U file2convert
```

As a general rule, use the man command to see how a command is used on your particular computer. When working with GODIVA, the transformation is automatically done on all the files.
dos2unix is available using the package manager of most of Linux distributions, but sometimes with the name `fromdos`.

A.2.4 Compilation problems

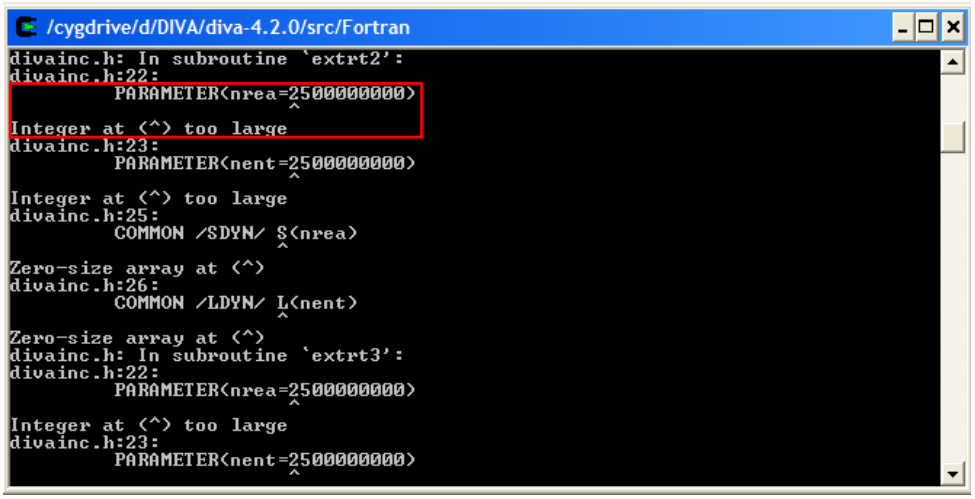


Figure A.6: Error message obtained during compilation.

A.2.5 Why do I get this error?

The array S defined in the various programs located in `./src/Fortran/Calc/` is too large to be handled by your compiler.

How to solve it?

You need to recompile the sources after reducing the values of parameter `nrea` in file `./src/Fortran/Calc/divainc.h`:

```
PARAMETER(nrea=150000000)
```

Then use script `divacompile` to get the new executables (see Section 1.3.1). If you get the same error message, reduce again the value of `nrea`.

A.2.6 Undefined references to NetCDF routines

Why do I get this error?

The NetCDF library, required for compiling of `netcdfoutput.f` and `netcdfoutput-field.f`, is not compatible with your compiler, or not found by the linker.

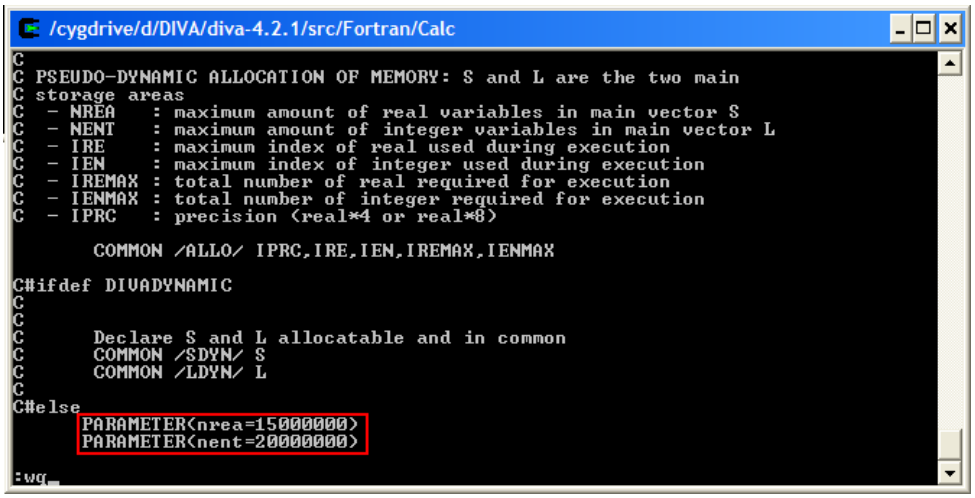


Figure A.7: Solution to the resource problem.

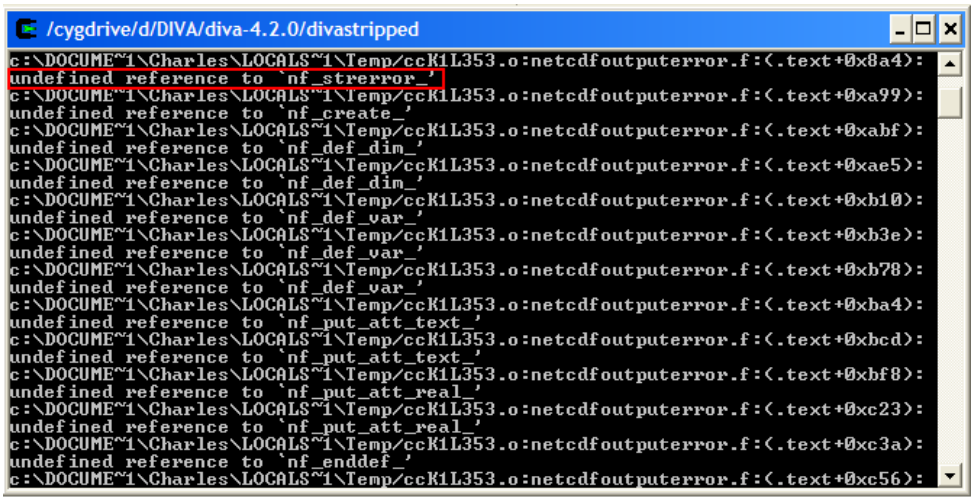


Figure A.8: Error message during execution of `divacomp` with gfortran.

How to solve it?

Make sure that `divacompileall` includes the appropriate link path.

If this is not sufficient, you will have to rebuild the NetCDF library corresponding to your operating system. Installation and compilation procedures can be at http://www.unidata.ucar.edu/software/netcdf/docs/netcdf-install/.

A.2.7 Resource temporarily unavailable

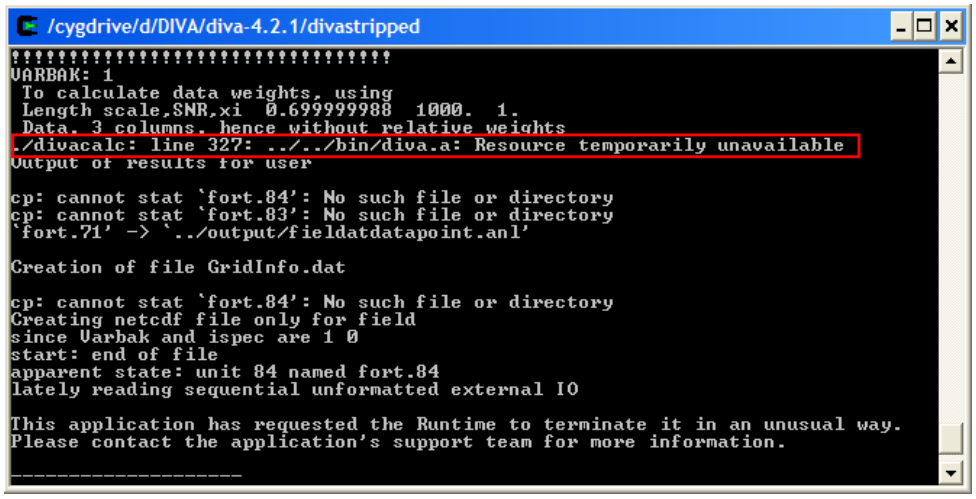


Figure A.9: Error message during the run of `divacalc`.

Why do I get this error?

The `diva.a` executable requires to much memory to work. This error comes from the operating system limitations.

How to solve it?

First try to cancel all unnecessary tasks running on your machine, possibly rebooting. This will clean up the system and free up resources. If this is not sufficient, the solution is the same as case A.2.4: recompile the sources after reducing the values of parameters `nrea` and `nent` in file `./src/Fortran/Calc/divainc.h`:

```
PARAMETER(nrea=25000000)
PARAMETER(nent=25000000)
```

If you get the same error message, reduce again the values of `nrea` and `nent`.

Note that maximal allowable values for these parameters depends on your compiler and system, so it is not possible to assign them with universal values.

A.2.8 Error of allocation

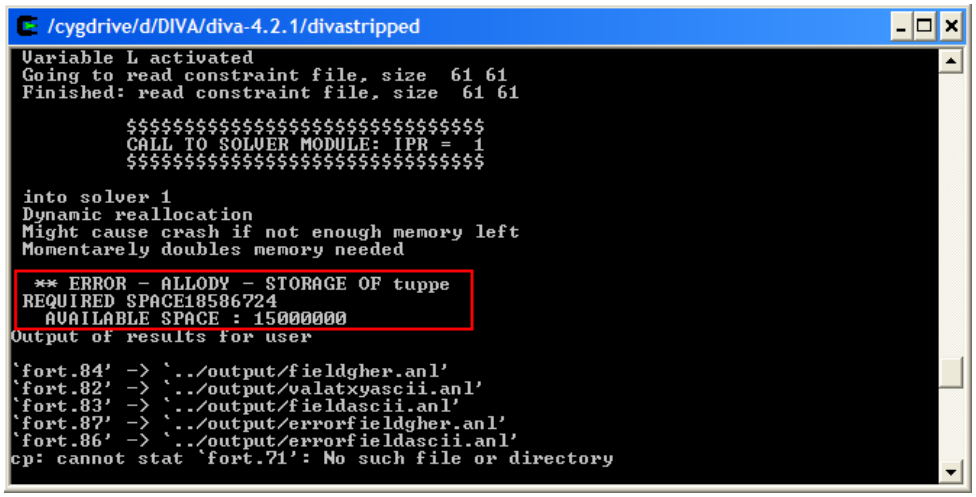


Figure A.10: Error message due to allocation problem.

Why do I get this error?

The memory allocation is not sufficient for the Diva to be executed in the case you consider. This message may appear either during the mesh generation (the required mesh is too fine considering the size of the domain) or during the resolution itself (i.e., `divacalc`).

How to solve it?

The solution is nearly the same as the previous case: you need to compile the source again, this time after increasing the values of `nrea` and `nent`.

Additional information ⋆⋆⋆

In some uncommon cases, you may not be able to find values of `nrea` and `nent` that will allow you to avoid both problems A.2.7 and A.2.8. In these cases, the recommended solution consists of:

1. Find the highest values of `nrea` and `nent` that allow you not to have message error A.2.8;
2. Generate a mesh with a value 3-5 times larger than the correlation length you want to use for the resolution; this can be done be simply editing file `./input/param.par`, changing the value of correlation length, and run `divamesh`;
3. Once the mesh is generated, edit again `param.par` and assign the correct value to the correlation length, and run an analysis with `divacalc`.

This procedure should help you to save memory otherwise used for the finite-element mesh. Working with a coarser mesh will not affect excessively your results.

A.2.9 Permission denied for execution of `diva.a`

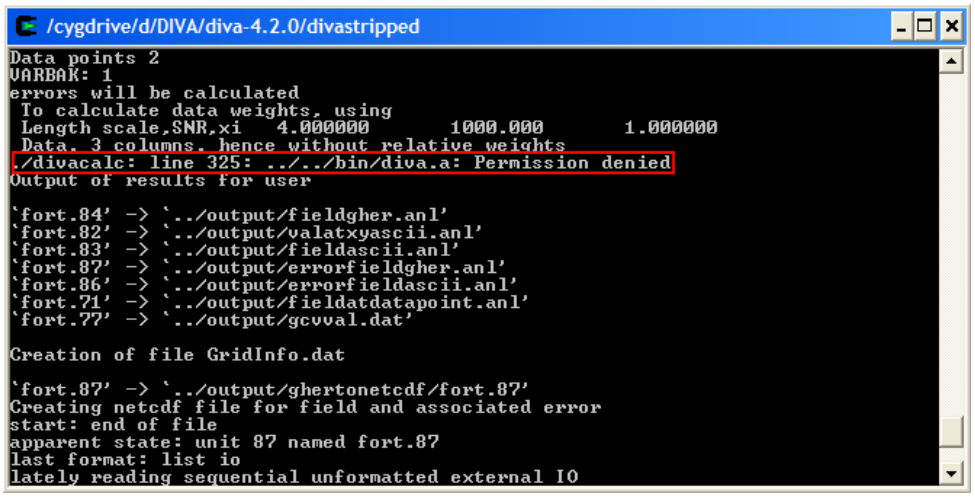


Figure A.11: Error message during execution of `divacalc` with gfortran.

Why do I get this error?

Although the compilation worked without any message error, `diva.a` cannot be executed. This problem seems to occur only with *gfortran* compiler under Cygwin. Actually the problem is not related to permission (command `chmod` will not solve the problem) but with compilation. As described in problem A.2.7, values of parameters `nrea` and `nent` shall be decreased and the sources recompiled.

How to solve it?

Same as problem A.2.7.

A.2.10 Problem with contour generation

See Fig. A.12.

Why do I get this error?

The number of contours created from a given topography (Section 7.2.2) is too high.

How to solve it?

Modify the first line of `contourgen.f` (located in `./src/Fortran/Mesh/`) and increase the value of `nm`:

```
parameter(nm=5000000)
```

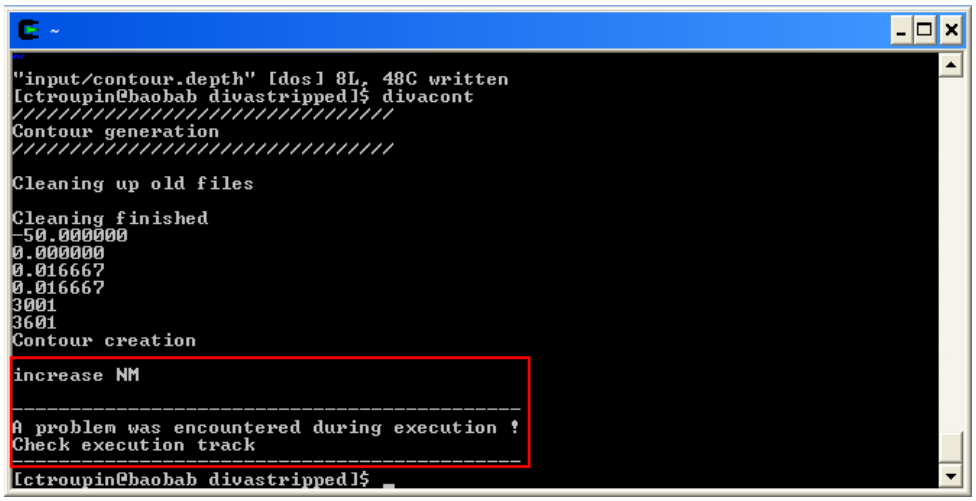


Figure A.12: Error message with contour generation.

Additional information

As the default value of `nm` is already large, you may also consider working with a topography with lower resolution. This should avoid the creation of of a great number of very small contours (e.g. Fig. A.13), which will not necessarily add quality to your analysis.

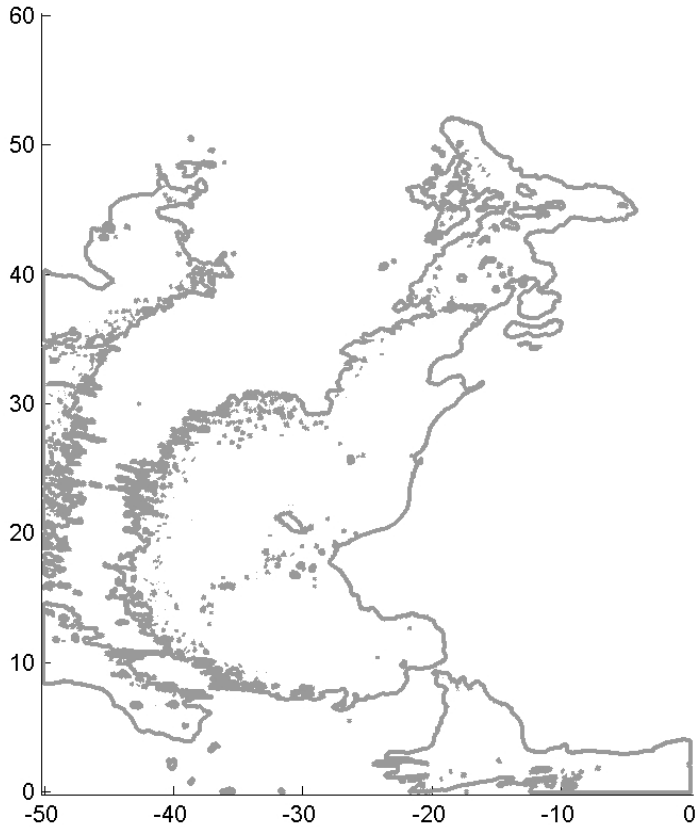


Figure A.13: Small contours created from DBDBV topography in the North Atlantic at 4500 m depth.

A.2.11 Analysis yields empty field

After the execution of `divacalc`, you get very small input files, with only one grid point.

Why do I get this error?

The most frequent reason is that the `param.par` file has been modified during the execution of (Generalised) Cross Validation and the process was interrupted before it ends, leaving a parameter file similar to A.14. Note that in order to save computational time, `nx` and `ny` are set to 1, since the analysis at every grid points is not necessary.

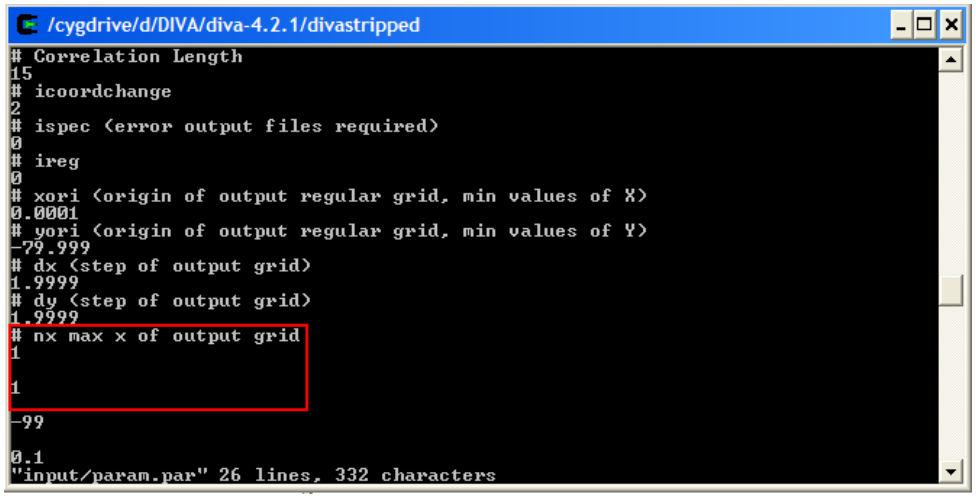


Figure A.14: File `param.par` resulting from an interruption of `divagcv`.

How to solve it?

Simply edit `param.par` to write the correct values of `nx` and `ny`, then run again `divacalc` (or `divadress`) to have an analysis on the desired grid.

A.2.12 Windows runs out of virtual memory during diva execution

Why do I get this error?

The problem arises probably because you have a computer with little RAM.

Diva uses a memory allocation for the largest problem encountered. This translates in Windows to a request of virtual memory of around 1.3 Gb. During execution, the real memory used can be much smaller than that and the problem actually fit in real memory, even if you have less than 1 Gb RAM.

The only problem is that if your Windows virtual memory (the swap file) is not big enough, Diva will not execute.

How to solve it?

The best solution would be to add real memory (your computer would benefit from it anyway), but to make Diva work you can simply increase the virtual memory of Windows

by changing the windows settings. As administrator:

```
my computer   right click
 -> properties  -> advanced -> performance
 -> settings -> advanced -> change
```

Put there a virtual memory (swap file) of 2 Gb (initial and maximum) and Diva should run.

Other solution consists of recompiling with lower `nrea` value (see problem A.2.4).

A.2.13 "Cannot move directory" ..."permission denied" messages

Why do I get this error?

1. An application has opened one or several files located in the directory you want to (re)move, so that it is impossible to perform the operation. 2. You are looking into diva temporary subdirectories with an explorer while running. In this case, an error message like this one can appear:

```
mv: cannot move 'output' to 'workexerr/output': Permission denied}
```

How to solve it?

Simply close the application(s) that open/explore the files of the concerned directory.

A.3 Solved problems

The following problems should not appear any more in the latest version of Diva. Should you encounter them, please contact us.

A.3.1 Jacobian matrix with null determinant

The value of the Jacobian determinant is zero (Fig. A.15).

Why do I get this error?

This messages comes from a problem in the mesh generation: some of the triangular elements are too deformed and generate a null value for the determinant. Then the solver cannot work, since it needs to inverse the Jacobian matrix.

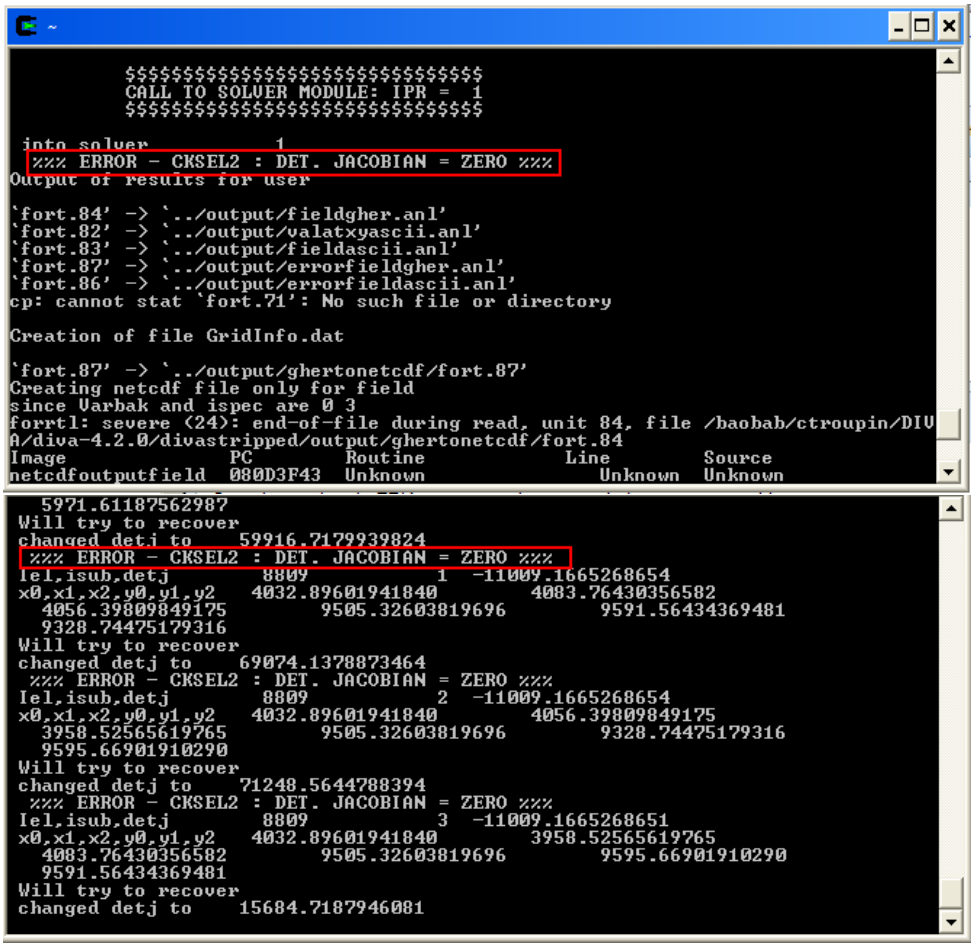


Figure A.15: Examples of Diva execution with problem with the Jacobian matrix.

How to solve it?

This problem was fixed in latest versions of Diva.

A.3.2 Analysed field with white stripes

The analysed fields has stripes of NaN values.

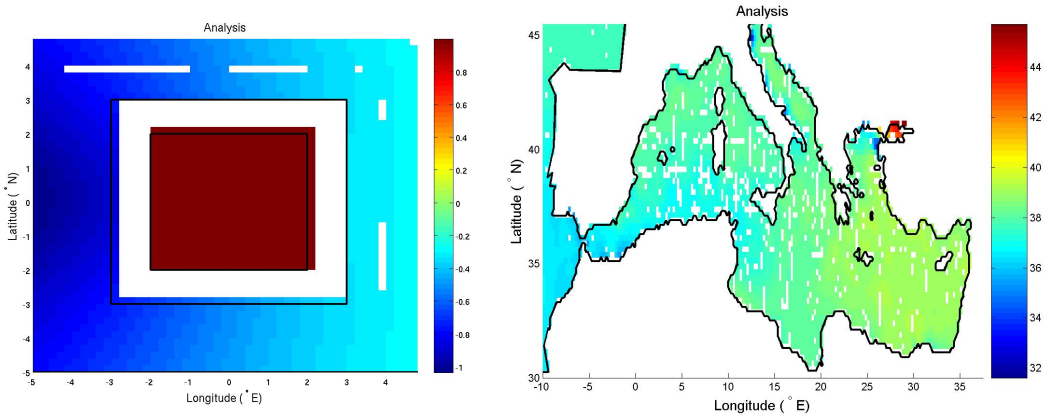


Figure A.16: Examples of Diva outputs with random zones of NaN.

Why do I get this error?

This problem comes from a too aggressive optimisation to create executable `diva.a`, although during the compilation, no warning or error was issued.

How to solve it?

This problem has been fixed in latest version of Diva. However, if you are still using older versions and get this kind of outputs, you can avoid them by changing the compilation flags and compile the source again. The recommended change is to use `'-O0'` flags instead of `'-O3'` (optimization flags) when compiling the sources located in the `Fortran/Calc/` directory.

A.3.3 "Corrupted data file" message

Why do I get this error?

This problem was observed when decimal numbers were written with commas instead of points.

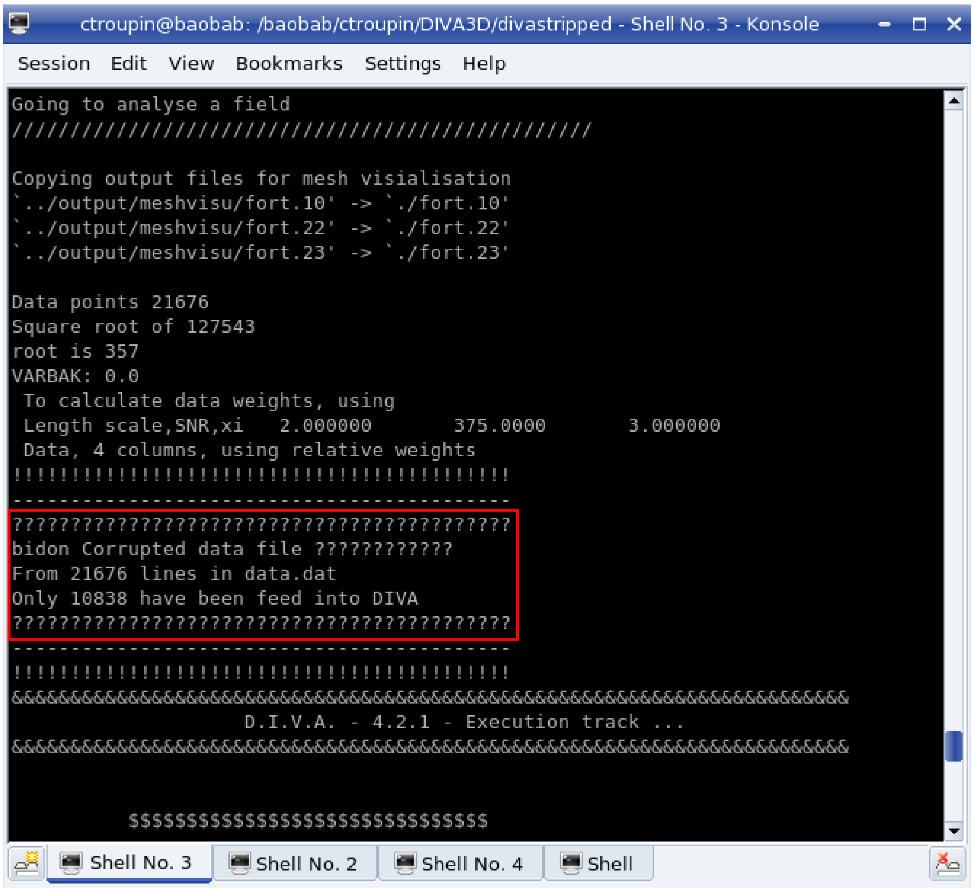


Figure A.17: Error message during the reading of the data file.

How to solve it?

Simply convert the decimal separator (e.g. using the commands described in the beginning of Chapter 6).

Additional information

The behaviour of `awk` is susceptible to change the points into commas when used in `awkfilter` or other routines. To fix the problem, simply replace

`gawk`

by

`LC_ALL=C gawk`.

Remark: in latest versions of the code, this bug was fixed by adding

`export LC_ALL=C`

in the scripts employing `awk`.

The engine of Diva is a set of Fortran subroutines driven by local input and output files (`fort.*`). This chapter is dedicated to the description of these programs, in order to allow the advanced user to adapt the code according to his needs.

Contents

B.1 Fortran code ⋆⋆⋆

The Fortran programs are sorted according to their purpose:

```
[Fortran] tree -d -L 1
.
|-- Calc
|-- Extensions
|-- Mesh
|-- NC
|-- NoPlplot
|-- Pipetest
|-- Plplot
|-- Stabil
`-- Util

9 directories
```

B.1.1 Calculation programs [src/Fortran/Calc]

The main file of the Fortran code is `diva.f`: this routine calls the subroutines enumerated below, in order to perform a Diva analysis:

mathpr.f : describes the mathematical problem.

topolo.f : describes the topology of the finite element grid.

meshgn.f : generates a square finite element mesh on a regular grid.

datapr.f : input of data to be fitted by spline smoothing.

bcondi.f : Dirichlet boundary conditions to be fixed.

constr.f : input of information for constraint implementation.

solver.f : builds and solves the global linear finite element system.

stores.f : storage of the solution.

esterr.f : estimates the analysis error (same grid as the analysis).

coord.f : coordinate change (longitude, latitude) to (x, y) and (x, y) to (longitude, latitude) if requested.

gcvfac.f : estimates the analysis error by generalized cross-validation.

dataqc.f : data quality check: estimates of expected data-analysis differences.

covar.f : calculation of Diva kernel for subsequent error fields.

Other routines related to Diva calculation:

allody.f : dynamical allocation of storage area in S or L vector.

bilinin.f : interpolates from a regular field into xt, yt; called in **constr.f**.

finca.f : finds in which region is one point.

optimi.f : subroutines used for the optimisation:

- **divesp.f**: subdivides the space for optimisation;
- **sizes2.f**: computes the size of the space for elements of type 2;
- **sizes3.f**: computes the size of the space for elements of type 3;
- **repel2.f**: distributes the elements of type 2 in kntc table;
- **repel3.f**: distributes the elements of type 2 in kntc table;
- **locpt2opti.f**: locates the (x, y) point in the structure (for ityp=2);
- **locpt3opti.f**: locates the (x, y) point in the structure (for ityp=3);
- **sortdopti.f**: sorts the data according to the sequence of elements;
- **qs2i1r.f**: quick Sort algorithm for **sortdopti** (from www.netlib.org);
- **calpsoopti**: computes pseudo data sets for error estimates;
- **fcorropti.f**: part of **calpsoopti**;
- **tabess.f**: tabulates the Bessel function for the calculation of error.

repeltest.f : called in datapr.f

shapef.f : evaluation of the shape functions at Gauss points.

utilit.f : utility routines.

uur.f : for the advection constraint.

uwrit2.f : writes the field $C(I, J, K)$.

varl.f : for variable correlation length.

vtools.f : various subroutines:

intsec: calculate center coordinates of quadrangular element;

istria: check if one point lies inside a triangle;

prskyh: print a vector to check.

B.1.2 Mesh programs [src/Fortran/Mesh]

Files related to the generation of coastlines:

contourcheck.f : check the format of an existing contour file (no repeated points, no crossing, contour not too fine).

contourgen.f : create contours based on topography;

coa2cont.f : go from ODV .coa files (see documentation of ODV) to Diva coast.cont files, using a resolution comparable to the specified gridded output of divacalc.

Files related to mesh generation:

generopt.f : generate a multi-connex 2D mesh with the *Delaunay triangulation*;

generopt4.f : same as generopt but in real*4 precision;

generopt8.f : same as generopt but in real*8 precision.

B.1.3 Pipetest [src/Fortran/Pipetest]

File piperw.f checks if *pipes* are supported by your Diva installation. Pipes support is automatically tested when you run divatest (Section 1.4). Issues with pipes were observed with some versions of the gfortran compiler.

B.1.4 Utilities [src/Fortran/Util]

alpha.f computes the values of α_0 and α_1.

calcest.f : from relative weight on data points (data file fort.44) and generalized cross validator value (available in ./output/gcvval.dat), produces the file containing the expected misfit value at data locations (fort.76), to be used by lookfor-outliers.a for outliers detection. Used in divaqcter.

calcestbis.f : from relative weight on data points (data file fort.44) and the trace of the analysis matrix (available in ./output/gcvval.dat) produces the file containing the expected misfit value at data locations (fort.76), to be used by lookfor-outliers.a for outliers detection. Used in divaqcbis.

calcmu.f computes the coefficient μ knowing the characteristic length L and the signal-to-noise ratio λ.

cverror.f : rms error by cross validation (called in divacvrand).

cverroraii.f : same as cverror.f but using the *missing-data lemma* (called in divacv).

cvtotalerror.f : sum of the different error contributions, in the resampling case (called in divacvrand).

datacheck.f : take the input data ./input/data.dat and eliminates all data that fall outside the bounding box of the contours (called in divadataclean).

datadiff.f : compute data anomaly (called in divaanom)

dbdb2diva.f : converts topography extracted from Navy website into Diva compatible format (Section 7.1.5).

gebco2diva.f : converts topography extracted from GEBCO website into Diva compatible format (Section 7.1.2).

findmin.f : from a list of values (SNR, GCV, data-variance) found in fort.11, tries to find by local parabolic interpolation the minimum of GCV and the place SNR where it is found.

Points do not need to be ordered. Output (fort.12) contains the expected value of λ in which GCV is minimal as well as the VARBAK value. Used in divagcv.

Called in divacv,divacvrand anddivagcv.

fitlsn.f : from the data file (fort.10) and information on coordinate change and reference field (fort.11), tries to fit the *Bessel covariance function* to the data covariance (called in divafit).

Outputs:
fort.66 contains the correlation length and an rough estimate of the signal-to-noise ratio;
fort.99 contains the data-covariance over all distances;
fort.98 contains the data covariance as a function of data-distance as well as the corresponding fit over distances up to the correlation length.

forgnuplot*.f consists in nine files for preparing the outputs to be viewed with the help of gnuplot(see Section 9.1).

griddef.f creates the file GridInfo.dat, of which the content is used for writing the NetCDF output.

lceleme.f computes the mesh characteristic length (called in divacck and divamesh).

lookforoutliers.f checks if there is outliers in the data provided for the analysis (called in divacalc, divaqcbis and divaqcter).

multiply.f does what its name says (called in divarefe).

subsampling.f creates a subsampling of the data (called in dvsample).

sumgrid.f performs the sum of two gridded fields in GHER format (called in divasumup).

sumup.f performs the sum element by element of two ascii files (called in divasumup).

topoprep.f makes easier the generation of the topography using a collection of local measurements (called in divatopo).

Remark: grid definition for users is based on an origin which is the first grid point. In the code, xori and yori are defined by x_i = xori $+i\Delta x$ (and is thus shifted one grid space to the left compared to the user origin). Input file fort.13 is modified from the param.par grid information by griddef.a accordingly, while GridInfo.dat contains the user grid as defined in param.par.

B.1.5 NetCDF output [src/Fortran/NC]

Three files allow getting an output in NetCDF format:
netcdfoutputfield.f, netcdfoutputerror.f, netcdfoutput.f.

The two first routines write the analysed and the error fields in two different NetCDF files: anlysed_field.nc and error_field.nc. The last programs generates results.nc which contains both the analysis and the error fields. The information required for the coordinates (xorigin, yorigin, dx, dy, nx, ny) are read from GridInfo.dat.

```
1
1
.5
.5
100
100
```

Example file B.1: GridInfo.dat

B.1.6 GUI programs [src/Fortran/Extensions]

The graphical interface requires some particular routines:

extract.f : interface to select or extract Data from MODB and MED formatted databases.

fem3d.f is based upon a mesh file and a bathymetry file (regular grid in GHER format); it creates a result file containing information to determinate if a mesh is in land or is sea, for a given depth.

concat.f is used to create the 3D file from the 2D files.

stiff.f generates the rigidity file (fort.60) in the 3D case.

mask.f masked the solution according to the bathymetry and the depth.

sum.f writes the sum of two fields (with same dimensions) in GHER format.

substref.f subtracts the reference field to the computed solution (only available when using the *semi-normed* reference field).

header2.f and visu.f are subroutines to visualize the data, the mesh and the solution (requires the PlPlot library). Two versions of visu.f are provided: one is located in diva-4.7.1/src/Fortran/PlPlot and the other in src/Fortran/NoPlPlot. The first can be compiled only if you have installed the PlPlotlibrary on your computer (for now, only under Linux).

B.2 Input and output files for the executables

This section describes the input and output files fort.* related to the executables or binaries, which are the files ending by .a and located in GODIVA_mm_yyyy/DIVA3D/bin/.

B.2.1 Mesh generation: generopt.a

Files readed as input

fort.10: coast file (identical to coast.cont), see example file with description, case of a square island in a square sea.

fort.11: the parameters required for the mesh generation.

Files produced as output

fort.22: contains the finite-element mesh, as described here:

1. the first part of the file has three columns: the first column gives the numbers of the nodes; the second and third ones give the $x-$ and $y-$coordinates of the nodes, respectively.
   Example first line indicates that node no. 1 is located in $(-1, -1)$.
2. the second part is composed of only one column, which indicates the numbers of the interfaces;
3. the last part has six columns: columns 1, 3 and 5 specify the line numbers where the coordinates of the triangle points can be found; columns 2, 4 and 6 specify the interfaces numbers of the considered element.
   Example the last line says that the last elements has its coordinates in lines 2, 3 and 5, *i.e.*, at has points $(1, -1)$, $(1, 1)$ and $(-0.3333333430.333333343)$; it also says that this element is composed of interfaces no. 13, 8 and 12.

```
1 -1. -1.
9 1. -1.
4 1. 1.
10 -1. 1.
7 -0.333333343 0.333333343
5
11
6
12
8
2
13
3
3 -6 4 -7 5 -8
4 -9 1 -10 5 -7
1 -11 2 -12 5 -10
2 -13 3 -8 5 -12
```

Example file B.2: fort.22

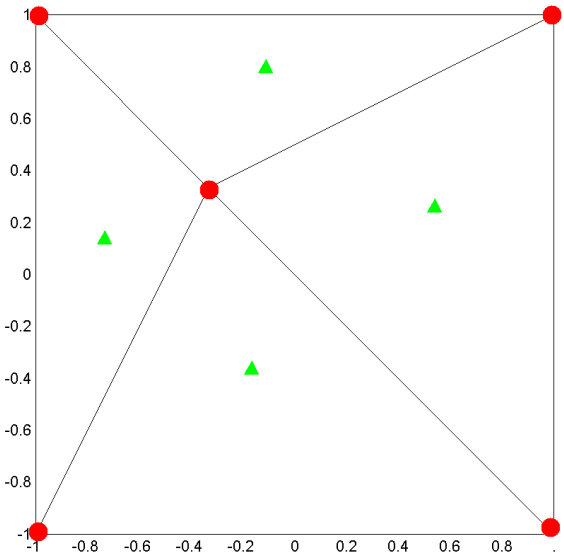


Figure B.1: Example of simple mesh corresponding to file `fort.22`.

`fort.23`: contains the topological parameters:

1. total number of vertex nodes (red dots);
2. total number of interfaces (black lines);
3. total number of elements (green triangles).

```
5
8
4
```

Example file B.3: fort.23

B.2.2 Diva interpolation: `diva.a`

Files read as input

`fort.10`: `divawork` organizer, defining which modules to use and how, including several parameters.

`fort.11`: finite-element mesh, copy of the `fort.22` produced by `generopt.a`.

`fort.12`: α_0 and α_1, calculated as:

$$\alpha_0 = \frac{1}{L^4} \quad \text{and} \quad \alpha_1 = \frac{2}{L^2}.$$

`fort.13`: characteristics of the regular output grid.

fort.20: data file; 4 columns: $|X|Y|data(X,Y)|\mu|$, where

$$\mu = 4\,\pi\,\frac{\lambda}{L^2},$$

with λ, the signal-to-noise ratio.

fort.79: coordinates where analysed field values are requested; 2 columns separated by space: $|X|Y|$.

fort.15: parameter `varbak`, variance of the background field, set as = 0 will avoid calculating error field.

```
coord 1
0
mathpr 1
2 -> ITYP
0 -> ISYM
2 -> IPB
topolo 1
158 -> Number of Vertex Nodes
426 -> Number of Interface Nodes
268 -> Number of Elements
datapr 1
1
solver 1
0
stores 1
1 -> 1 if normal or semi-normed final, otherwise 3
esterr 1
stopex
```

Example file B.4: fort.10

```
0.0001 -> alpha0
0.02 -> alpha1
```

Example file B.5: fort.12

```
0 0 -> xorigin, yorigin
1 1 -> dx, dy
100 100 -> nx, ny
-99999 -> Exclusion Value
```

Example file B.6: fort.13

```
90 90 1 12.5663706
90 80 1 12.5663706
90 70 1 12.5663706

                                        ...


16 30 2 12.5663706
16 20 2 12.5663706
16 10 2 12.5663706
```

Example file B.7: fort.20

Files produced as output

fort.71: field value at data points given in fort.20, ascii format.

fort.72: error value at data points given in fort.20, ascii format.

fort.73: error at points given in fort.79, ascii format.

fort.82: field value at points given in fort.79, ascii format.

fort.83: field on regular grid, ascii format.

fort.84: field on regular grid, gher format.

fort.86: error field on regular grid, ascii format.

fort.87: error field on regular grid, gher format.

B.2.3 Detrending calculation: detrend.a

The execution of detrend.a will create a new ./input/data.dat.

Files read as input

fort.88: original data file.

fort.89: analysis at data points.

Files produced as output

fort.90: modified data file with data detrended by groups and classes.

trends.1.dat: trends for classes of group 1.

trends.2.dat: trends for classes of group 2.

...

C VADEMECUM

The DIVADEMECUM is a four-page summary of the commands and the input/output files you have to deal with when using Diva.

Contents

C.1 Scripts and actions

Table C.1: DIVADEMECUM: Diva in- and outputs. When not specified differently, input files are from directory `./input` *and output files are placed in directory* `./output`*. Script* `divarefe` *takes the same inputs as* `divacalc` *while* `divaanom` *and* `divasumup` *use no other user-provided files than the other scripts. Brackets* `[ ]` *enclose optional files or parameters. Ex.* `[-r]` *will replace an input file by the outputs from the scripts.*

Input	Action Execution	Output
mycase/input/*	load new case divaload mycase	./input/*
topo.dat param.par	make gridded topography divatopo [-r]	TopoInfo.dat [./input/TopoInfo.dat] topo.grd [./input/topo.grd]
topo.asc topo.gebco	use dbdb or gebco topography dbdb2diva [-r] gebco2diva [-r]	TopoInfo.dat [./input/TopoInfo.dat] topo.grd [./input/topo.grd]
TopoInfo.dat topo.grd [contour.depth]	make contours divacont [-r]	coast.cont.* [./input/coast.cont.*]
param.par coast.coa	use ODV contours divacoa2cont [-r]	coast.cont [./input/coast.cont]
param.par coast.cont	check hand–made contours divacck [-r] [-v]	coast.cont.checked [./input/coast.cont]
../*/fort.*	clean up directories divaclean	
data.dat coast.cont [./output/fieldatdatapoint.anl]	eliminate useless data divadataclean [f_{min} f_{max}]	./input/data.dat
data.dat coast.cont [./output/fieldgher.anl]	bins of data coverage divadatacoverage [-n] [-r]	DATABINS*.dat RL*.dat
param.par data.dat	estimate L and S/N divafit [n] [-r]	covariance.dat covariancefit.dat paramfit.dat param.par.fit [./input/param.par]
param.par coast.cont [coast.cont.dens]	make FE mesh divamesh	divamesh outputs
gcvsampling.dat param.par data.dat divamesh outputs [Uvel.dat,Vvel.dat UVinfo.dat, constraint.dat] [RL.dat, RLinfo.dat]	optimise S/N by cross–validation divacv [-r] divacvrand ns nt [-r] divagcv [-r]	gcv.dat gcvsnvar.dat gcvval.dat param.par.gcv [./input/param.par]
param.par data.dat divamesh outputs [Uvel.dat,Vvel.dat UVinfo.dat, constraint.dat] [RL.dat, RLinfo.dat] [valatxy.coord]	make analysis divacalc	GridInfo.dat field*.anl error*.anl *.nc [valatxyascii.anl]
param.par data.dat ./output/meshvisu/* [Uvel.dat,Vvel.dat UVinfo.dat, constraint.dat] [RL.dat, RLinfo.dat]	perform full quality control divaqc	outliers.dat outliers.normalized.dat
param.par data.dat divacalc outputs	perform simple quality control divaqcbis	outliersbis.dat outliersbis.normalized.dat
param.par data.dat divacalc outputs	perform simple quality control divaqcter	outlierster.dat outlierster.normalized.dat
./output/*	make some plots divagnu [f_{min} f_{max}]	./gnuwork/plots/*
./output/*	save results divasave mycase	mycase/outut/*

C.2 Workflow

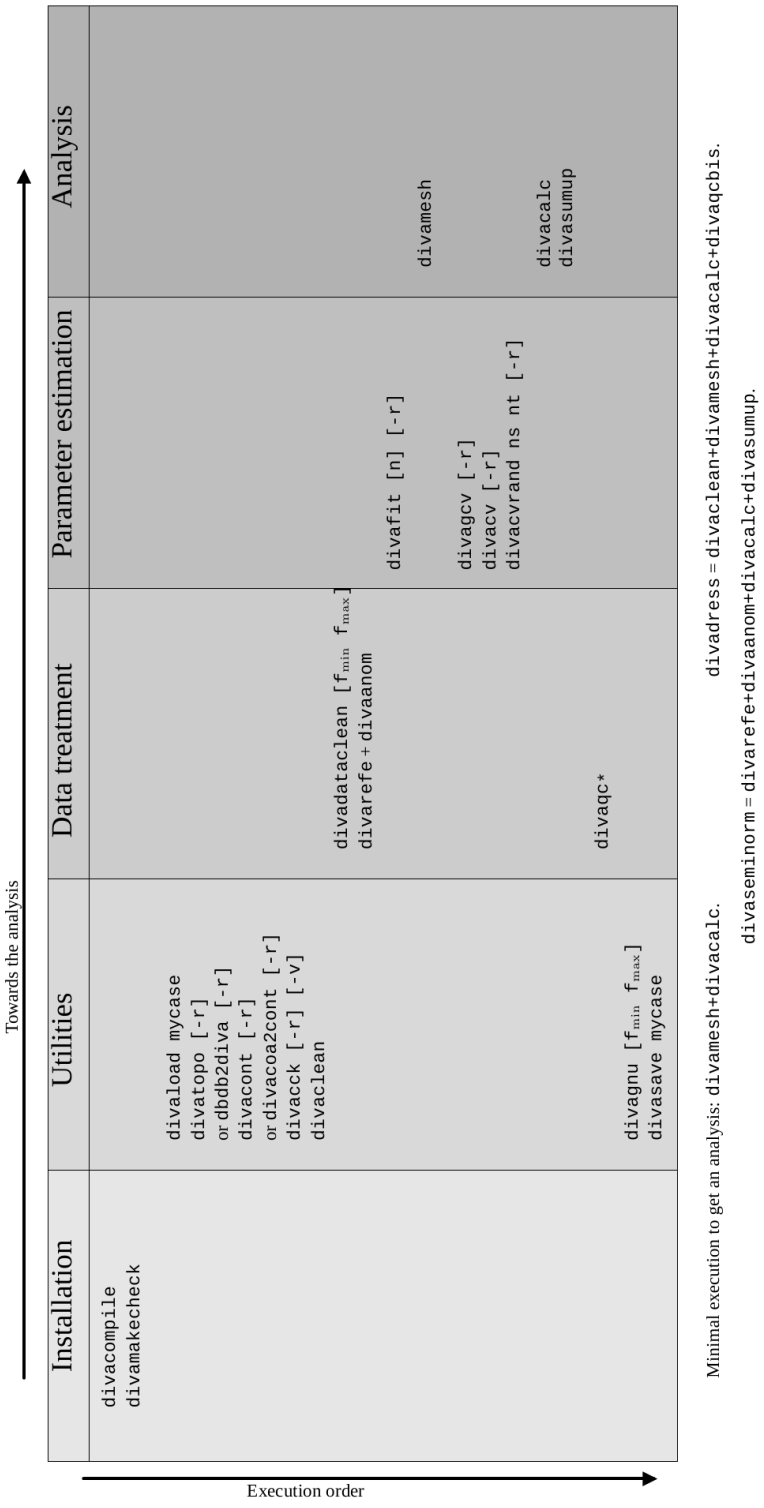


Figure C.1: Scripts used in the command-line version of **Diva**; *optional arguments are between* `[]`.

C.3 Input files

```
# Correlation length (in units of data, if degrees: S-N)
1
# icoordchange (-xscale, 0=none, 1=degtokm, 2=sin projection)
0
# ispec (error output files required)
7
# ireg (subtraction of reference field 0: no, 1:mean, 2:plane)
0
# xori (origin of output regular grid, min values of x)
-4.999
# yori (origin of output regular grid, min values of y)
-4.999
# dx (x-step of output grid)
0.1999
# dy (y-step of output grid)
0.1999
# nx number of x points of output grid
51
# ny number of y points of output grid
51
# valex (exclusion value)
-9999.0
# snr signal to noise ratio
10
# varbak variance of the background field
1
```

param.par file content. Parameters are self-explaining, except for error output specification. `ispec=0` means no error field requested; add +1 for a gridded error field, +2 for error at data location and +4 for error at coordinates defined in valatxy.coord. From there if you want

- error based on real covariance: `ispec` ← `-ispec`
- error based on real covariance with boundary effect: `ispec` ← `-ispec-10`
- poor man's error estimate (quick and underestimated error field): `ispec` ← `ispec+10`

(ex: `ispec=12` makes a poor man's error estimate at data locations)

```
-5  22 34.8
-2  19 36.1
...
```

data.dat file content. Simple ascii file with `x,y,val` and optional fourth column containing the relative weight on the data (large value = high confidence).
topo.dat is just a special case where the third column represents depth (positive for sea values).

```
100 10
```

constraint.dat file content.
First value = weight on advection constraint, second value=diffusion coefficient in advection/diffusion equation.

```
0.01
0.03
0.1
0.3
1
3
10
30
100
```

gcvsampling.dat file content. A list of trial values for the signal-to-noise ratio used in cross validation tools.

```
1000
750
500
400
300
200
100
0
```

contour.depth file content with depths for contours and subsequent analysis.

```
0
10
0.1
0.2
101
51
```

*info.dat file describing the gridding parameters of binary gridded files such as Uvel.dat, topo.grd, RL.dat, fieldgher.anl, errorfieldgher.anl. Here first grid point in $(0, 10)$, with steps $(0.1, 0.2)$ and 101×51 grid points. Look at examples how to read/write binary files with Fortran or Matlab

C.4 Output files

```
0.50E+01 1131 0.16E+02 0.43E+02 0.38E+02 0.37E+02 0.13E+00
...

 flag    ident   x   y   dataval  analysis expected-misfit
```

outliers*.dat Sorted outliers, from most suspect to least suspect. Column 1: outlier indicator (larger than 3 suspect), following columns: data identifier, x and y coordinates, original data value, analysed data value, expected misfit.

```
Correlation length (in degrees latitude)
  3.69890785
 Signal to noise ratio
  0.902823746
 VARBAK
  16.7839489
 For information: correlation length in km is  412.962524
```

paramfit.dat Self explaining output from `divafit`. When option `[-r]` is used with `divafit`, an adapted param.par will be placed in `./input`.

```
 S/N
  1.99764168
 VARBAK
  1.14215052
```

gcvsnvar.dat Self explaining output from `divacv, divagc, divacvrand`. When option `[-r]` is used with cross validation, an adapted param.par will be placed in `./input`.

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