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DIVAnd training: producing ocean climatologies with Jupyter notebooks

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Software

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Summary

The DIVA-workshops project consists of a set of Jupyter notebooks, focused on the creation of gridded fields from in-situ observations using `DIVAnd`. `DIVAnd` is a software tool, written in Julia, which performs interpolation in an arbitrary number of dimensions.

The notebooks address the different stages of oceanographic climatology generation: data reading and preparation, extraction of the topography and creation of a land-sea mask, setting of the spatial resolution and the time periods, estimation of the analysis parameters, analysis and creation of the metadata.

The target audience is broad as it includes: data analysts, who wish to create climatologies; physical oceanographers, who want to grid their observations for visualisation and potentially for quality control, and programmers, who want to include DIVAnd interpolation in a larger workflow involving other processing steps.

Statement of need

The gridding of in-situ measurements is a common task in oceanography. It consists of the generation of one or several fields on a regular grid, using the information contained in a set of observations, generally sparsely distributed. The combination of such fields, produced at different depths and for different time periods, is often referred to as a climatology.

This gridding problem is not new and many methods have been developed in recent decades. One of the most widespread methods is Optimal Interpolation (Bretherton et al., 1976; Gandin, 1966), where analytical functions are used to specify a first guess error covariance. Since then, the method has been adapted and improved, yet it cannot easily address the decoupling of water masses separated by a physical obstacle.

DIVA (Data-Interpolating Variational Analysis; Troupin et al. (2012)) is comparable to optimal interpolation, but it takes coastlines, sub-basins and advection into account. Mathematically, the method is based on the minimization of a cost function which includes different constraints, typically the closeness to observations and the regularity (or smoothness) of the gridded field. DIVA, written in Fortran, was based on a finite-element solver and limited to two-dimensional applications. Climatologies were obtained by assembling 2D fields produced at specified depths and time periods.

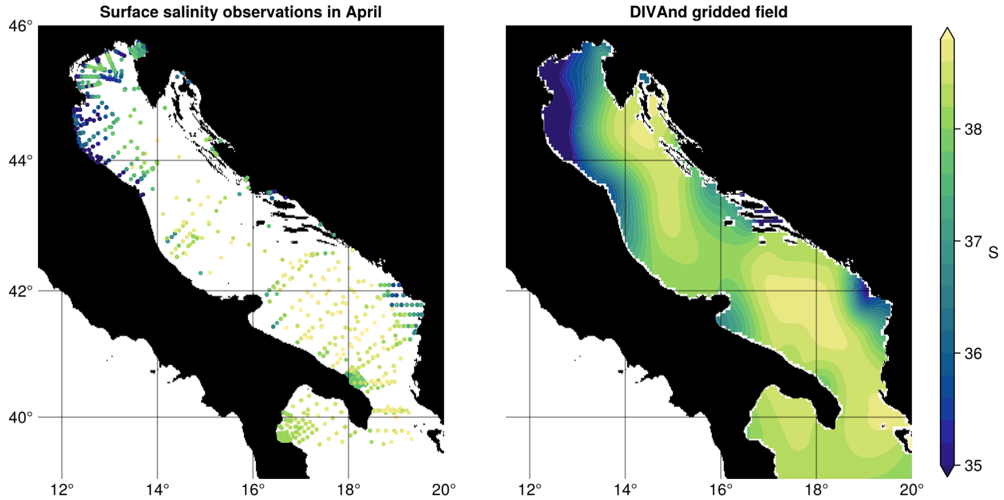

Figure 1: Example of salinity measurements and the corresponding analysed field.

`DIVAnd` (DIVA in n dimensions) is based on the same mathematical idea (the minimization of a cost function) but extended to an arbitrary number of dimensions, typically longitude, latitude, depth and time (Barth et al., 2014). The code was first rewritten so that it could run on MATLAB and GNU Octave. Its performance was further improved thanks to the transition to the Julia language (Bezanson et al., 2017).

Without reviewing the full development history of the gridding and interpolation algorithms, we highlight two specific aspects that are adequately addressed by DIVAnd (and DIVA) with respect to existing techniques:
1. The management of large datasets: the computation time is almost independent of the number of observations, making it possible to perform gridding with millions of data points.
2. The consideration of natural boundaries (coastlines, bottom topography) during the interpolation: the artificial mixing of water masses that are geographically close but separated by a physical obstacle is avoided.

The `DIVAnd` code is published on GitHub along with its documentation and examples, and the underlying theory has been published in Barth et al. (2014). However, in order to ensure that users are able to create their own climatologies, with a relatively new programming language, additional teaching resources were necessary. This is the main motivation behind the creation and the maintenance of the Diva-Workshops repository.

The DIVAnd learning module

The story

The first DIVA workshop was organized in Liège, Belgium, in 2006, as part of the European project Seadatanet (Schaap & Lowry, 2010). The goal was to teach users how to create climatologies by applying the DIVA (the two-dimensional, Fortran version) on their own dataset. Those training sessions were organized yearly until 2016 and allowed for the creation of regional climatologies, published as part of European initiatives such as SeaDataNet or EMODnet (Martín Míguez et al., 2019).

Taking advantage of the Jupyter interface (Kluyver et al., 2016) and the transition to Julia for the new version of DIVAnd, a set of notebooks was created as the primary resource

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for the user training. The first DIVAnd workshop took place in April 2018 in Liège. Since then, other training events were organised and the training material is regularly used as the basis for the creation of gridded products for EMODnet Chemistry (Giorgetti et al., 2018). The choice of the Jupyter notebooks format was motivated by the interactivity and the step-by-step, documented approach.

Participant feedback is particularly valuable. It not only guides the development of new functionalities in the DIVAnd source code, but also the creation of new notebooks describing specific workflows (for instance the consideration of geostrophy) or the use of particular functions (for instance the use of an advection constraint in the interpolation).

Goal of the module

The goal of the training material module is twofold:
1. to provide users with a basic knowledge of Julia, meaning they are not only capable of reading the code presented in the notebooks, but also able install new modules, write basic functions for processing or create basic plots.
2. to ensure that users are able to create their own products (i.e., climatologies) by combining their own datasets with those from other sources (for instance the World Ocean Database) and setting the analysis parameters according to their region of interest.

Julia syntax is similar to other widespread languages, for instance MATLAB, yet some peculiarities have to be explained to make sure users can take advantage of its full functionality.

Instructional design

The notebooks have been organized by sub-folders according to their objectives:
1. Introduction: brief introduction to the Julia language and to the Jupyter notebooks, how to deal with netCDF files (reading and writing) and how to generate figures (maps, sections, …).
2. Pre-processing: preparation of the input required by DIVAnd (grid, time periods, bathymetry, observations) and estimation of the main analysis parameters (correlation length and noise-to-signal ratio). Code fragments dealing with various file formats (CSV, netCDF, TIFF, …) are also provided to help users work with the most frequent types of data.
3. Analysis: creating of gridded fields with DIVAnd, the influence of the analysis parameters, and interpolation with different coordinate systems.
4. Advanced topics: this folder contains less frequently used notebooks, dealing with the generation of density maps, relative correlation length, background fields, and advection constraints.

Since the notebooks require input data files (mainly bathymetry and observations) to be executed, we ensure that those files are available from a public file server and can be downloaded locally whenever necessary.

Following our experience with users, for the creation of plots, the Makie module (Danisch & Krumbiegel, 2021) (along with GeoMakie for the maps) was selected to replace PyPlot along with Cartopy (Met Office, 2010 - 2015) for the maps, which is based on the Python Matplotlib module (Hunter, 2007). Indeed, the import of PyPlot in the notebooks often generated errors on user machines, due to the sensitivity to the operating system and the pre-existing Python installation(s).

Users and applications

The user community mainly consists of scientists, data analysts and experts. This diversity implies that the content has to be comprehensive and tailored to ensure users without any prior experience with Julia or Jupyter are able to run and modify the notebooks.

Among the applications, we highlight de EMODnet products (Webb et al., 2025). Other recent applications include the creation of climatologies and gridded fields for sea surface height (Doglioni et al., 2023) temperature and salinity (Shahzadi et al., 2021) and nutrients (Belgacem et al., 2021).

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