multi-Risk sciEnce for resilienT commUnities undeR a changiNgclimate

Codice progetto MUR: **PE00000005** – CUP F83C22001660002

Deliverable title: Radar constrained integrated simulation for oil spill and contaminant dispersion.

Deliverable ID: DV 4.4.3

Due date: 30/11/2024

Submission date: 30/11/2024

AUTHORS
Fabio Giordano (OGS); Federica Adobbati (OGS); Stefano Querin (OGS); Cosimo Solidoro (OGS); Alberto Guadagnini (UNIMI)

1. Technical references

Project Acronym	RETURN
Project Title	multi-Risk sciEnce for resilienT commUnities undeR a changiNg climate
Project Coordinator	Domenico Calcaterra UNIVERSITA DEGLI STUDI DI NAPOLI FEDERICO II domcalca@unina.it
Project Duration	December 2022 – November 2025 (36 months)

Deliverable No.	DV4.4.3
Dissemination level*	PU
Work Package	WP 4.4 - Multi risk assessment and proof of concepts
Task	T 4.4.3 - Integrated modelling, uncertainty analysis, inverse modelling and uncertainty reduction
Lead beneficiary	POLIMI
Contributing beneficiary	OGS

* PU = Public

PP = Restricted to other programme participants (including the Commission Services)

RE = Restricted to a group specified by the consortium (including the Commission Services)

CO = Confidential, only for members of the consortium (including the Commission Services)

Document history

Version	Date	Lead contributor	Description
0.1	30.092024	Alberto Guadagnini (OGS)	First draft
0.2	25.10.2024		Critical review and proofreading
0.3	20.11.2024		Edits for approval
1.0	30.11.2024		Final version

2. Abstract

The accurate and reliable simulation of oil spills and, in general, of contaminant dispersion at sea strongly depends on the realistic reconstruction of ocean dynamics, with particular focus on marine currents. Therefore, the quality of velocity fields (and turbulent parametrizations) derived from remote sensing measurements and/or numerical models is crucial when dealing with advection/diffusion problems. Integrating these data sources can leverage the strengths of different approaches, reducing the intrinsic flaws of each method alone (e.g., data gaps for measurements, model uncertainties for numerical simulations).

In particular, sea surface current observations from the high-frequency (HF) radar array deployed in the Gulf of Trieste can be assimilated into general circulation models to improve their accuracy. In this study, we used an “indirect” approach, with the aim of smoothing the assimilation update: the information obtained from measurements is propagated to the model via the atmospheric forcing by estimating the wind stress that drove the observed currents, rather than by directly modifying the velocity fields. Then, the updated wind forcing is applied to the model.

Two methods are outlined in the present report: the first one follows a physics-driven path, searching for solutions to the equations that relate wind to currents, and then performing a classic data assimilation scheme to update the atmospheric forcing. The second one is based on novel machine learning techniques, by finding relationships between wind and currents directly from the available data, both synthetic (from simulations) and observational (from HF radars).

The assimilated wind forcing will be then fed into the model, with the goal of improving its skill in terms of describing and forecasting the circulation in the Gulf of Trieste, with impacts on many applications, the most straightforward being better capabilities for tracking oil spills or other transported contaminants.

3. Table of contents

List of Tables

List of Figures

4. HFR surface currents assimilation to improve model skill

4.1 Estimating wind stress from observed marine currents

4.1.1 Motivation

Data assimilation is a technique adopted to modify the trajectory of a model, meant as a mathematical description of reality, by incorporating observations and trying to get as close to them as possible, while also keeping the model dynamical evolution.

The aim of this work is to assimilate the information contained in measured sea surface currents into an oceanographic model. However, instead of directly assimilating the current velocity, the objective here is to estimate the wind forcing that drives the observed currents and then update the atmospheric fields that are fed into the numerical model. This should, on one hand, "smooth out" the assimilation effect, as the new information is passed to the simulated fields indirectly via the wind forcing; furthermore, the model internal dynamics transfer the information from the surface to the ocean interior, a task otherwise to be implemented in the assimilation method. On the other hand, this approach could also be potentially way less expensive in terms of computational costs, since some assimilation techniques, when applied to large and complex models, are very computationally demanding.

4.2 Physics-driven assimilation in the Gulf of Trieste

4.2.1 Navier-Stokes equations and simplifications

In physical oceanography, the equations of motion are made of a set of partial differential equations (Navier-Stokes (NS) equations [1]):

$$\left(\frac{\partial}{\partial t} + \overline{V}\cdot\overline{\nabla} + \overline{f}\wedge\right)\overline{V} = \overline{g} - \frac{1}{\varrho}\overline{\nabla}P + \overline{\nabla}\cdot\left(\nu\overline{\nabla}\,\overline{V}\right)$$

with $\overline{V} = u\overline{x} + v\overline{y} + V_z\overline{z}$ velocity field, ϱ density, f Coriolis parameter, $\overline{g}$ gravitational acceleration, P pressure and ν kinematic viscosity. These equations are coupled with the continuity equation (for uncompressible flows) and the equations of state for temperature and salinity (to close the system). Once initialized and subjected to appropriate boundary conditions (at the surface, bottom and sides), these equations describe the evolution of the flow field in a geophysical context.

In the Gulf of Trieste, the NS equations can be simplified by means of a scale analysis: given the typical values for the quantities involved, some terms of the equations can be neglected. By assuming the hydrostatic balance, the vertical velocity component is set to zero; as for the horizontal scale, by neglecting the advective term (approximately one order of magnitude smaller than the time derivative) and the horizontal components of the diffusive term, one obtains:

$$\left(\frac{\partial}{\partial t} + \overline{f}\wedge\right)\overline{V}_h = -\frac{1}{\varrho}\overline{\nabla}P + \frac{\partial}{\partial z}\left(\nu\frac{\partial}{\partial z}\,\overline{V}_h\right)$$

By invoking the geostrophic balance, the velocity is decomposed in a constant, vertically uniform component, which balances the pressure gradient with the Coriolis force, resulting finally in:

$$\left(\frac{\partial}{\partial t} + \overline{f}\wedge\right)\overline{V}_h = \frac{\partial}{\partial z}\left(\nu\frac{\partial}{\partial z}\,\overline{V}_h\right)$$

4.2.2 Unsteady Ekman equation: analytical solution

By defining $w \doteq u + iv$ the system reduces to a single partial differential equation, akin to the widely studied heat equation:

$$\left(\frac{\partial}{\partial t} + if\right)w = \frac{\partial}{\partial z}\left(\nu\frac{\partial}{\partial z}w\right)$$

To close the problem, initial conditions (ICs) and boundary conditions (BCs) are required: for the former $w(z,\, t=0) = w_0(z)$ while for the latter $w(z=-h,t) = 0$ (no-slip condition at the bottom) and $\frac{\partial}{\partial z}w(z=0,t) = \frac{1}{\varrho\nu}\tau(t)$ (wind stress $\tau(t) = \tau_x(t) + i\tau_y(t)$ forcing the sea surface).

A final approximation consists of assuming that the kinematic viscosity is uniform along the vertical dimension: $\nu(z) = \nu$. This is the same assumption made by Ekman [2] to derive his relationship between wind stress and currents in the surface boundary layer in steady conditions: the obtained equation is a non-stationary extension to the same problem.

Given the analogy to the heat equation, the solution strategy is borrowed from the extensive theory developed for it (see, for example, [3]): the complex velocity field is split into two terms $w = w_1 + w_2$, the first solving the problem for the given initial conditions and setting the boundary conditions to zero, the second solving with the given BCs and setting the ICs to zero.

By separation of variables, the equation for w_1 is readily solved:

$$w_1(z,\, t) = \sum_{n=0}^{\infty} A_n \cos(k_n z)\exp(-(if + \nu k_n^2)t)$$

with

$$A_n = \frac{1}{h}\int_{-h}^{0} w_0(z)\cos(k_n z)\,dz\,,\; k_n = \frac{\pi}{2h}\left(n + \frac{1}{2}\right)$$

As expected, if the viscosity is zero the formula reduces to inertial oscillations, with frequency equal to the Coriolis parameter.

The equation for w_2, instead, can be solved following a procedure similar to [4], except that here the bottom depth is finite; in this regard, this equation is a particular case of the classification presented by [5].

By applying a Laplace transform from the time domain to the frequency domain the equation becomes

$$(s + if)\widetilde{w} = \nu\left(\frac{\partial^2}{\partial z^2}\widetilde{w}\right)$$

Imposing the boundary conditions, we obtain the solution in the frequency domain as:

$$\widetilde{w} = \widetilde{G}\widetilde{\tau} = \frac{1}{\varrho\nu q}\frac{\sinh\big(q(z+h)\big)}{\cosh(qh)}$$

with

$q = \sqrt{\frac{s+if}{\nu}}$.

Finanziato dall'Unione europea NextGenerationEU | Ministero dell'Università e della Ricerca | Italiadomani PIANO NAZIONALE DI RIPRESA E RESILIENZA

The solution in the time domain is therefore a time convolution of the wind stress with the transfer function $G(z,t)$that, from inverse Laplace transform as in [6], is equal to

$$G(z,t) = \frac{1}{\varrho h} \exp(-ift)\, \theta_1\left(\frac{z+h}{2h}; \frac{\nu t}{h^2}\right)$$
$$= \frac{2}{\varrho h} \sum_{n=0}^{\infty} (-1)^n \exp\left(-\left(if + \nu\left(n+\frac{1}{2}\right)^2 \left(\frac{\pi}{h}\right)^2\right) t\right) \sin\left(\pi\left(n+\frac{1}{2}\right)\frac{z+h}{h}\right)$$

where $\theta_1(a,x)$is the first Theta function [6].

To check against the Ekman stationary limit, constant wind stress $\tau(t) = \tau_0\left(1+\frac{i}{2}\right)$ is considered. This gives, convolving it with the transfer function:

$$\lim_{t\to\infty} w(z=0,t) = \frac{2\tau_0}{\varrho h} \sum_{n=0}^{\infty} \frac{1-\exp(-(\omega_n + if)t)}{\omega_n + if} \longrightarrow \frac{2\tau_0}{\varrho h} \sum_{n=0}^{\infty} \frac{1}{\omega_n + if}$$

with $\omega_n = \nu\left(n+\frac{1}{2}\right)^2 \left(\frac{\pi}{h}\right)^2$.

Figure 1 shows this asymptotic behaviour as a function of the bottom depth; for deep waters the angle between the wind stress and the surface currents (lower panel) reaches 45° to the right, as expected from the infinite depth theoretical formulation by Ekman. The values adopted are reported in Table 1.

Table 1 – Values adopted for the asymptotic behaviour of the solution

$\boldsymbol{\nu}$ m² s⁻¹	$\boldsymbol{\varrho}$ kg m⁻³	$\boldsymbol{f}$ s⁻¹	$\boldsymbol{\tau_0}$ N m⁻²	$\boldsymbol{h}$ m
$1.0\cdot10^{-2}$	$1.0\cdot10^{3}$	$1.0\cdot10^{-4}$	$1.6\cdot10^{-1}$	$2.0 \div 100.0$

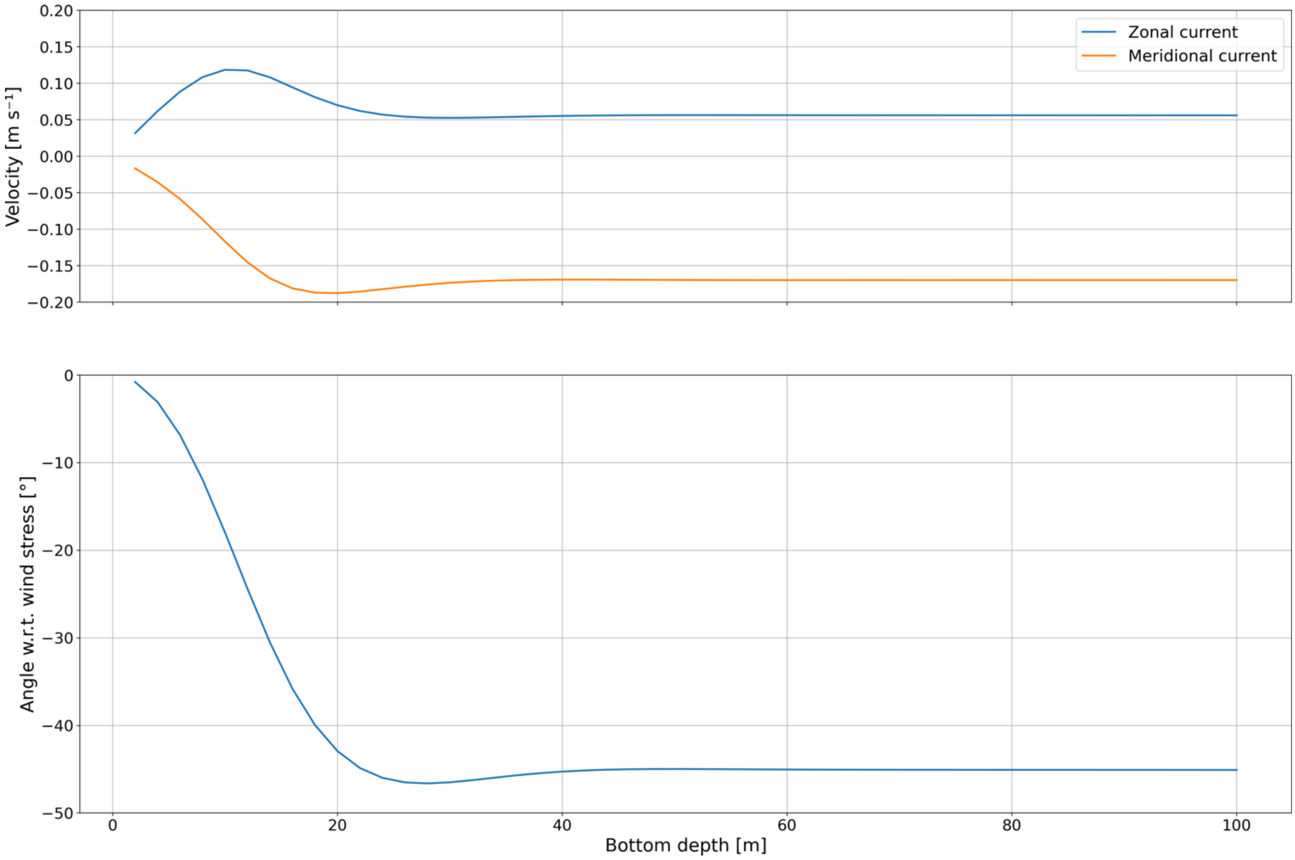

Figure 1 – Asymptotic behaviour of wind-driven surface currents velocity and direction

We performed a comparison between the analytical result and an idealized numerical simulation obtained by using the MITgcm [7] model. The simulation was set up in a double periodic box, with horizontal extension and resolution approximately equal to the operational forecasting system running in the Gulf of Trieste (https://medeaf.ogs.it/got). We imposed a flat bathymetry (25 m deep), uniform vertical viscosity (set to $5 \cdot 10^{-3}$ m^2 s^{-1}) and initial conditions with null velocity. The simulation was run with the full Navier-Stokes equations in a non-hydrostatic configuration; therefore, it explicitly considers the terms neglected in the previous derivation by scale analyses arguments. Atmospheric forcings were realistic, obtained from weather forecasts, except for the wind, set as a constant, uniform value of 11.5 m s^{-1} westerly.

Figure 2 shows the results, comparing the topmost (0 to 0.5 m) layer's velocities: the solid line represents the numerical model solution, averaged over horizontal blocks of around 1.5 km, representing the HF radar resolution. Some discrepancies are noted, with instabilities due to vertical shear present in the MITgcm simulation, but most of the dynamics is captured by the unsteady Ekman model, confirming its usefulness in estimating the sea surface response to wind stress.

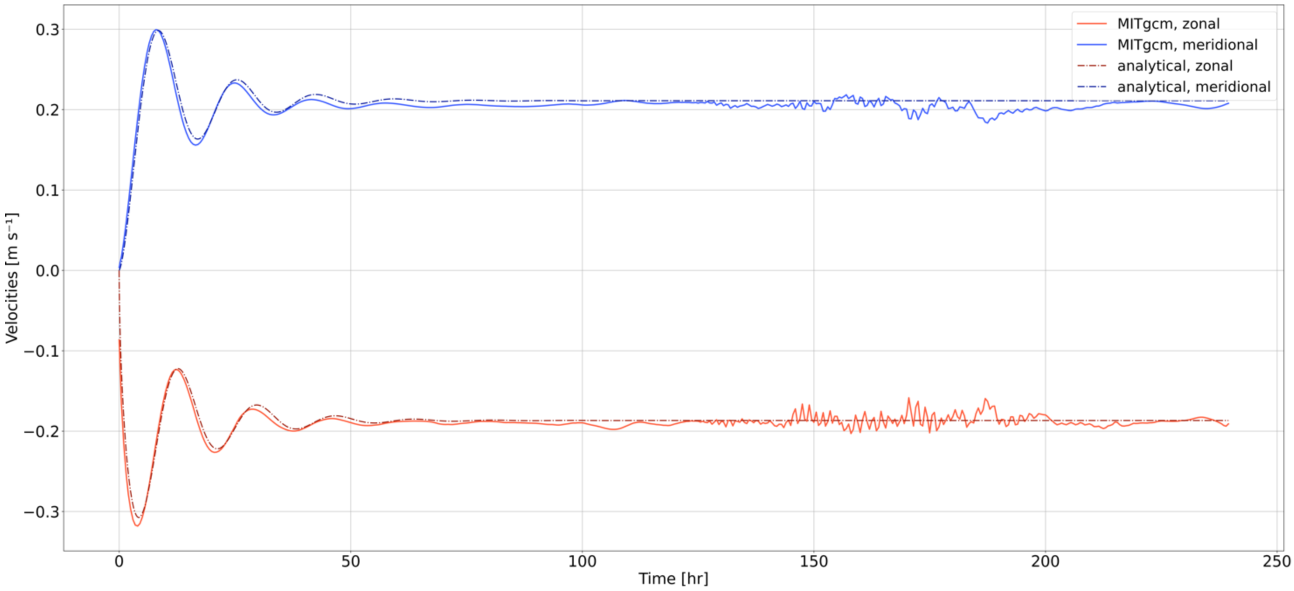

Figure 2 -– Time evolution of the surface solution of wind-driven currents from numerical and analytical models

4.2.3 4D-Var

Given this analytical, yet approximate, result, it could be possible to obtain an estimate (analysis) of the wind stress field starting from a background information (e.g. wind stress as forecasted by a weather model) and observations, in this case given by the WERA high frequency radar (HFR) array deployed along the Gulf of Trieste [8] (Figure 3), that allows for measurements of sea surface currents, via data assimilation.

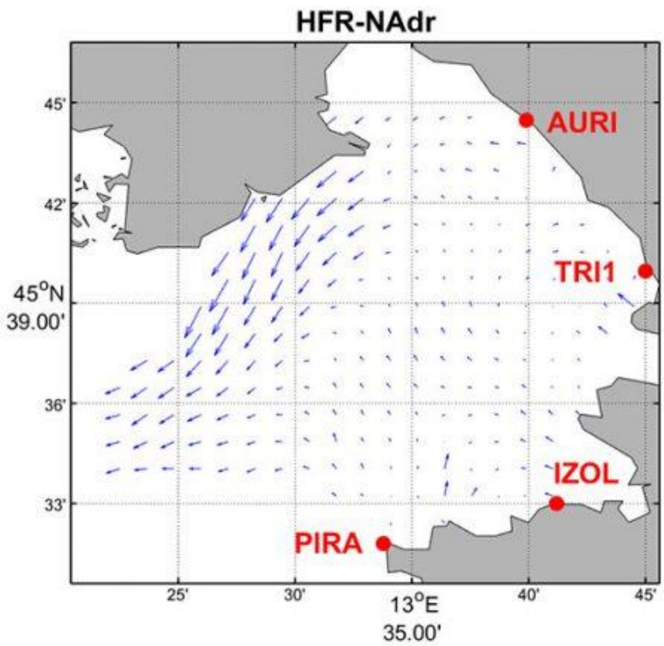

Figure 3 – Position of the Gulf of Trieste HF radar array and geographical coverage

One possible method to perform this task is the variational data assimilation, which consists of minimizing a so called cost or objective function that considers both background and observations: calling a, b, o the analysis, background and observation values respectively, the function to be defined in general has the form

$$J = (a-b)^T C_b^{-1}(a-b) + (a-o)^T C_o^{-1}(a-o)$$

with C_b, C_o covariances associated to the background and observation errors. The result of this minimization process, the analysis, gives the best "fit" between data and model.

Since the analytical surface currents are the result of a time convolution, the minimization must consider the temporal dimension: the approach is usually referred to as 4D-Var [9], due to the inclusion of the fourth dimension (time) other than the three spatial ones.

Work is now in progress to define and compute the covariances needed for the cost function, as well as to choose the minimization approach (e.g. gradient descent).

4.3 Machine learning-driven assimilation in the Gulf of Trieste

4.3.1 State of the art

The method described in the previous section aims to estimate the wind stress that better "fits" the observed currents, relying on the analytical solution of the physical problem of wind driven circulation. To do so, some approximations have been invoked to linearise the relationships between wind stress and ocean currents.

Conversely, one can try to keep the nonlinear behaviour of fluid motion and estimate the wind stress directly from the data. Machine learning techniques could be applied to integrate HF radar data in the prediction of sea surface currents.

Indeed, the use of machine learning for data assimilation tasks is becoming more and more common [11] and, in earth science applications, there is often the specific requirement that outputs satisfy physical constraints. In [10] and [12], the authors describe several methods that has been used to bring together physics and machine learning, with a specific focus on geoscience applications. However, there is not yet much literature about the specific task we are tackling.

In [13], the authors use a Multi-Layer Perceptron to predict sea surface currents at the global scale given sea surface height (SSH), surface wind stress (zonal and meridional), sea-surface temperature (SST, θ), sea-surface Salinity (SSS), latitude and longitude. In [14] the authors present a deep learning model to reconstruct satellite data. Inpainting problems like this, have some similarity with the one that we propose to tackle, since radar data may also have some missing information that we need to reconstruct in our final product.

For our case-study, in order to obtain data consistent with our physical knowledge, we are exploring the possibility to integrate machine learning with numerical models: in particular, we want to use neural networks to predict wind conditions starting from the radar data, in order to minimize the difference between the radar data and the output of the numerical model, given the newly computed wind field.

To test our idea, we plan to first train a surrogate model of the numerical general circulation model, which provides sea surface current fields starting from wind fields, by using the sea surface current data produced by the model as ground truth. This step is useful, since the neural network can provide a result way faster than the physical model (see for example [10]).

A second phase consists in training a neural network to produce a wind field starting from HF radar data, computing the loss function as the difference between radar data and the output of the surrogate model produced in the first phase.

5. Conclusions

The two approaches outlined in this work will be carried out in parallel, offering the opportunity to cross-check their skill and identifying strengths and weaknesses of each one of them.

With respect to classic data assimilation techniques, machine learning methods are usually computationally cheaper. On the other hand, they do not directly use physical knowledge, making their results more difficult to interpret and trust. It will be interesting to compare the two alternative approaches, also with the aim to study how they can be integrated with each other.

The final goal of this work is to assimilate the estimated wind stress into a numerical model of the Gulf of Trieste, to improve its skill in simulating surface circulation, with applications in hindcasting and forecasting of passive tracer dispersion. Figure 3 (modified from [15]) shows the comparisons between the positions of real drifters released in the Gulf and the corresponding virtual drifters, transported by currents measured by the radar array (panel a) and simulated by a high-resolution general circulation model (panel b). After time periods of the order of one day, the separation between real and virtual (model derived) drifters grows to a spread of around 10 km; the spread between real and HFR-derived drifters is instead lower, especially referring to the tails of distributions. By assimilating the radar observations, it will be possible to reduce the error in tracers transport in the model, allowing for better forecasting of potentially harmful contaminants, such as oil spills from the tankers reaching the Port of Trieste, helping policymakers and stakeholders in the decision-making process.

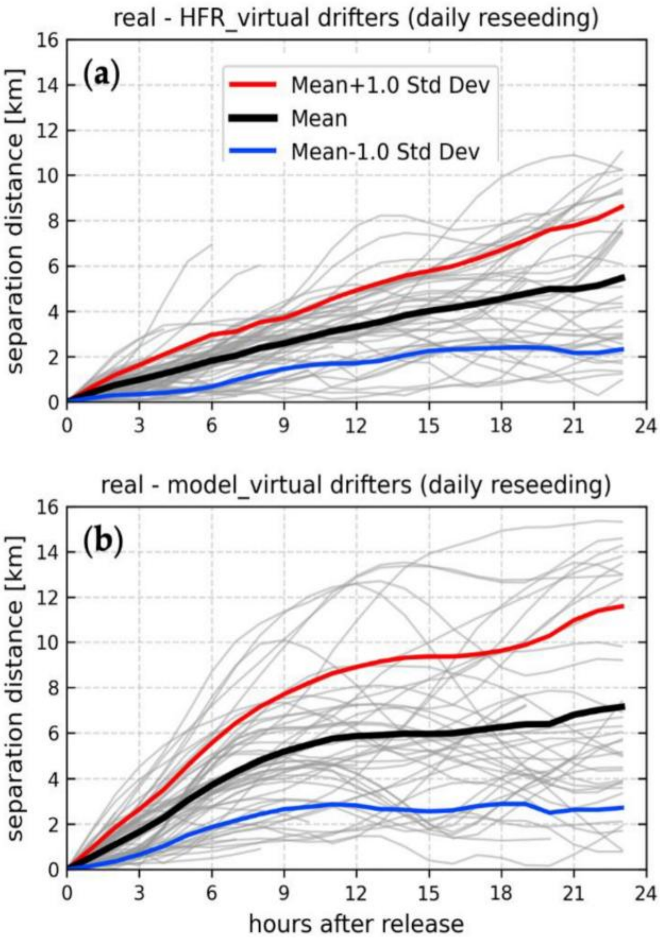

Figure 4 – Difference in the position of real and virtual drifters: a) virtual HFR drifters, b) virtual model drifters (modified from [15])

6. References

[1] Cushman-Roisin, B. and Beckers, J.M. "Introduction to Geophysical Fluid Dynamics: Physical and Numerical Aspects". Elsevier Science (2011), 9780120887590

[2] Ekman, V.W. "On the influence of the Earth's rotation on ocean currents". Ark. Mat. Astr. Fys. (1905), 2, 1–36.

[3] "Exact Analytical Conduction Toolbox", https://mme-exact.unl.edu/

[4] Madsen, O.S. "A realistic model of the wind-induced Ekman boundary layer". J. Phys. Oceanogr. (1977), 7, 248–255. doi:10.1175/1520-0485(1977)007<0248:ARMOTW>2.0.CO;2.

[5] Lilly, J. M., and Elipot, S. "A Unifying Perspective on Transfer Function Solutions to the Unsteady Ekman Problem". Fluids (2021), 6(2), 85. https://doi.org/10.3390/fluids6020085

[6] Oberhettinger, F. and Badii, L. "Tables of Laplace Transforms". Springer Berlin, Heidelberg (1973). https://doi.org/10.1007/978-3-642-65645-3

[7] Adcroft A., Campin J.-M., Doddridge E., Dutkiewicz S., Evangelinos C., Ferreira D., Follows M., Forget G., Fox-Kemper B., Heimbach P., Hill C., Hill E., Hill H., Jahn O., Klymak Losch M., Marshall J., Maze G., Mazloff M., Menemenlis D., Molod A. and Scott J. "MITgcm Documentation" (2024). https://doi.org/https://doi.org/10.5281/zenodo.1409237

[8] HFR-NAdr (High Frequency Radar NAdr network). OGS, NIB, ARSO, & ARPA FVG. (2023). European HFR-Node. https://doi.org/10.57762/8RRE-0Z07

[9] Carrassi A., Bocquet M., Bertino L., Evensen G. "Data assimilation in the geosciences: An overview of methods, issues, and perspectives". WIREs Clim Change. (2018). 9:e535. https://doi.org/10.1002/wcc.535

[10] Willard, J, Jia, X., Xu, S., Steinbach, M., Kumar, V. "Integrating physics-based modeling with machine learning: A survey." ArXiv preprint arXiv:2003.04919 1.1 (2020): 1-34.

[11] Cheng, S., Quilodrán-Casas, C., Oula, S., Farchi, A., Liu, C., Tandeo, P., Fablet R., Lucor, D., Iooss, B., Brajard, J., Xiao, D., Janjic, T., Ding, W., Guo, Y., Carrassi, A., Bocquet, M., Arcucci, R. "Machine learning with data assimilation and uncertainty quantification for dynamical systems: a review." IEEE/CAA Journal of Automatica Sinica 10.6 (2023): 1361-1387.

[12] Shijie, J. and Zheng, Y., Solomatine, D. "Improving AI system awareness of geoscience knowledge: Symbiotic integration of physical approaches and deep learning." Geophysical Research Letters 47.13 (2020): e2020GL088229.

[13] Anirban. S. and Abernathey, R. "Estimating ocean surface currents with machine learning." Frontiers in Marine Science 8 (2021): 672477.

[14] Barth, A., Brajard, J., Alvera-Azcárate, A., Mohamed, B., Troupin, C., Beckers, J. M. "Ensemble reconstruction of missing satellite data using a denoising diffusion model: application to chlorophyll a concentration in the Black Sea." EGUsphere 2024 (2024): 1-26.

[15] Querin, S., Cosoli, S., Gerin, R., Laurent, C., Malačič, V., Pristov, N., Poulain, P-M. "Multi-Platform, High-Resolution Study of a Complex Coastal System: The TOSCA Experiment in the Gulf of Trieste". Journal of Marine Science and Engineering (2021). 9(5):469. https://doi.org/10.3390/jmse9050469