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| 1 | Neural prediction of Lagrangian drift trajectories on the sea surface |
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ABSTRACT: We simulate Lagrangian drift on the sea surface and investigate deep learning ap-8 proaches to address the shortcomings of current model-based and Markovian approaches, particu-9 larly concerning error propagation and computational complexity. We present a novel deep learn-10 ing framework, referred to as DriftNet, inspired by the Eulerian Fokker-Planck representation of 11 Lagrangian dynamics. Through numerical experiments for simulated and real drift trajectories on 12 the sea surface, we illustrate the effectiveness of DriftNet compared to existing state-of-the-art 13 schemes. We also delve into the influence of diverse geophysical fields, whether derived from 14 models or observations, used as inputs by DriftNet on drift simulation. Our objective is to assess 15 the amount of dynamic information required to accurately simulate realistic trajectories. 16

SIGNIFICANCE STATEMENT: We propose a novel Deep Learning model, DriftNet, for con-17 ditional generation of Lagrangian trajectories on the sea surface. Our model is based on Eulerian 18 Fokker-Planck formalism and can be conditioned by multiple geophysical fields. We highlight the 19 overall over-performance of DriftNet compared to the baseline model-based and learning-based 20 approaches. We put in evidence the capacity of the proposed method to extract pertinent infor-21 mation from various geophysical fields, both from modeled and observed data. We highlight the 22 significant impact of the observed sea surface height when combined to sea surface currents in the 23 quality of the generation of Lagrangian trajectories. 24

1. Introduction

The modeling and simulation of Lagrangian drift on the sea surface holds relevance for various 26 applications such as the tracking of plastics and other debris Maximenko et al. (2012), the study 27 of algae and plankton dynamics Son et al. (2015), or the prediction of future locations of drifting 28 objects that is crucial for search and rescue operations Breivik et al. (2013). Furthermore, the 29 analysis of Lagrangian drifts serves as a valuable tool for diagnosing ocean numerical models in 30 their capability for reproducing small-scale dynamics Barron et al. (2007). However, reproducing 31 realistic Lagrangian trajectories on the sea surface poses a significant scientific challenge within 32 operational oceanography Röhrs et al. (2021). 33

From a methodological standpoint, we can distinguish three main categories of approaches 34 for Lagrangian drift simulation: model-based approaches Liubartseva et al. (2018); Zambianchi 35 et al. (2017), probablistic data-driven schemes Visser (2008), and more recent deep learning tech-36 niques Botvynko et al. (2023); Jenkins et al. (2023). Model-based approaches involve a sequen-37 tial advection process based on known sea surface velocity fields Lange and van Sebille (2017). 38 However, small errors in the underlying velocity fields or velocity fields without very fine spa-39 tial resolution may lead to unrealistic Lagrangian trajectories Callies et al. (2021). This often 40 impedes their operational usuefulness due to significant uncertainties in the forecasting and recon-41 struction of sea surface dynamics, especially regarding mesoscale ocean dynamics Prants et al. 42 (2017). Due to their sequential nature, these schemes also face scalability challenges when simu-43 lating large ensembles of drift trajectories. By contrast, probabilistic data-driven schemes usually 44 leverage first-order Markovian models and naturally account for uncertainties in the drift process. 45

However, they are primarily suited for relatively coarse space-time resolutions. Extending these 46 schemes to capture fine-scale patterns poses a challenge Fine et al. (1998). For these two first cat-47 egories, the simulation of the Lagrangian drift relies on location-wise velocities at each time step, 48 which may only be applicable for smooth velocity fields. Deep Learning has recently emerged as 49 a novel class of numerical tools for the learning-based simulation of movement patterns. We may 50 cite applications to pedestrians Korbmacher and Tordeux (2022), seabirds Roy et al. (2022), cars 51 Jiang et al. (2019) or maritime vessels Nguyen and Fablet (2024). These applications leverage 52 state-of-the-art recurrent neural networks, such as Long Short-Term Memory (LSTM) networks 53 Yu et al. (2019), as well as deep generative schemes Goodfellow et al. (2020); Roy et al. (2022); 54 Ma et al. (2019); Gan et al. (2020); Julka et al. (2021); Paz et al. (2021). Most of these studies can 55 be regarded as neural extensions of probabilistic Markovian schemes. 56

In this context, we present an innovative Deep Learning framework, referred to as DriftNet, for 57 simulating Lagrangian trajectories at the sea surface. The proposed neural model takes as input 58 geophysical fields characterizing the ocean dynamics in a spatio-temporal region and produces 59 the associated Lagrangian trajectory. Our approach is fully-convolutional and features a spatially-60 explicit latent representation, drawing inspiration from Eulerian Fokker-Planck representations of 61 drift processes Botvynko et al. (2023). From numerical simulation datasets, we demonstrate Drift-62 Net to outperform state-of-the-art neural schemes for the simulation of Lagrangian trajectories, 63 including when considering degraded sea surface velocities. The application to real sea surface 64 drifters' datasets further supports the relevance of DriftNet to improve the simulation of Lagra-65 gian drift on the sea surface compared with model-driven simulations. This last experiment also 66 illustrates how DriftNet can exploit additional data sources, besides sea surface velocities, here 67 satellite-derived sea surface height fields. 68

This paper is organized as follows: section 2 focuses on the problem description; we introduce DriftNet in section 3 and the considered experimental setup in section 4; section 5 details our results and section 6 discusses key aspects of this study.

72 2. Problem statement

In the context of Lagrangian fluid dynamics¹, one may describe a flow by following the motion of an ensemble of individual particles Davis (1991). In order to describe the flow in the Lagrangian

¹From now on, the Lagrangian notations are presented with \rightarrow symbol, and the Eulerian notations are in **bold**.

⁷⁵ framework, an ordinary differential equation defines the particle's trajectory :

$$\frac{\partial \vec{r}(\vec{r_{t_0}},t)}{\partial t} = \vec{v}(\vec{r_{t_0}},t) = \mathbf{u}(\vec{r}(t),t)$$
(1)

⁷⁶ where $\vec{r}(\vec{r}_{t_0},t)$ and $\vec{v}(\vec{r}_{t_0},t)$ are respectively the position and velocity at time *t* of the particle situated ⁷⁷ at \vec{r}_{t_0} at t = 0, and $\mathbf{u}(\vec{r}(t),t)$ is the Eulerian velocity of the underlying flow given position $\vec{r}(t)$ and ⁷⁸ time *t*. Classical model-driven approaches simulate Lagrangian drift dynamics through explicit ⁷⁹ time and space integration methods such as Runge-Kutta 4. Thus, the integration of eq.(1) leads ⁸⁰ to :

$$\vec{r}(\vec{r_{t_0}}, t + \Delta t) = \vec{r}(\vec{r_{t_0}}, t) + \int_t^{t + \Delta t} \vec{v}(\vec{r_{t_0}}, \tau) \mathrm{d}\tau$$
(2)

The sequential nature of this equation introduces important propagation of errors when the underlying velocities are not accurately known Callies et al. (2021).

Interestingly, we can also derive an Eulerian formulation of Lagrangian dynamics. Through Fokker-Planck formalism Visser (2008), we can generalize eq.(2) to the time propagation of the Probability Density Function (PDF) of the moving particle as follows:

$$\frac{\partial}{\partial t}p_{\vec{r}}(x,t) = -\frac{\partial}{\partial x}[\mu(x,t)p_{\vec{r}}(x,t)]$$
(3)

where *x* represents spatial position in the Eulerian framework, *t* the time, $p_{\vec{r}}(x,t)$ the PDF of the particle at position \vec{r} and $\mu(x,t)$ a drift field. In our case, this drift term relates to the underlying Eulerian velocity field $\mathbf{u}(x,t)$. Solving eq.(3) relies on a time integration scheme from the initial PDF $p_{\vec{r}}(x,t=0) = p_{\vec{r}_0}(x,0)$.

Here, we rely on this Eulerian Fokker-Planck representation of Lagrangian dynamics to explore
 convolutional neural architectures for the simulation of individual drift trajectories.

3. DriftNet for Lagrangian drift simulation

This section introduces the mathematical framework and the architecture of the proposed neural network model, called DriftNet, along with the considered learning scheme.

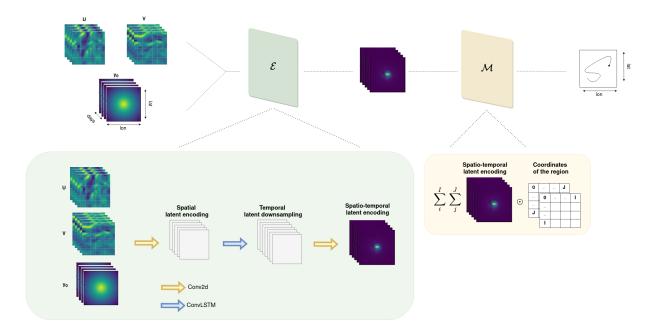


FIG. 1: **DriftNet architecture:** The input geophysical fields over 9-day (here zonal U and meridional V components of the velocity field) coupled to the initial spatio-temporal positional encoding y_0 are first passed to the encoding block \mathscr{E} and output a spatio-temporal latent encoding. The second block of DriftNet \mathscr{M} maps this latent representation to a 1D trajectory, *i.e.* a time series of positions on the sea surface.

95 a. Proposed neural scheme

- Given a spatial domain of interest \mathscr{D} defined as a regularly-gridded domain of size $I \times J$, we
- ⁹⁷ define the associated sequence of velocity fields $\mathbf{u} = {\mathbf{u}_{t_0}, \mathbf{u}_{t_0+\Delta}, \dots, \mathbf{u}_{t_0+K\Delta}}$ from time t_0 to $t_0 +$
- ⁹⁸ $K\Delta$, where Δ is the time sampling and K the number of time steps, and the trajectory of a particle as
- ⁹⁹ a time series of locations $\vec{r} = {\vec{r}_{t_0}, \vec{r}_{t_0+\Delta}, \dots, \vec{r}_{t_0+K\Delta}}$ in \mathscr{D} from t_0 to $t_0 + K\Delta$, where \vec{r}_{t_0} corresponds ¹⁰⁰ to the initial position of the particle.
- Inspired by Fokker-Plank eq.(3), we consider the following latent representation for a simulated Lagrangian drift \vec{r} :

$$\begin{cases} \mathbf{y} = \mathscr{E}(\mathbf{u}, \mathbf{y}_0) \\ \vec{r} = \mathscr{M}(\mathbf{y}) \end{cases}$$
(4)

where $\mathbf{y} = \{\mathbf{y}_{t_0}, \mathbf{y}_{t_0+\Delta}, \dots, \mathbf{y}_{t_0+K\Delta}\}$ is a space-time-explicit latent embedding of \vec{r} , and $\mathbf{y}_0 = \mathbf{y}_0$

¹⁰⁴ { $\mathbf{y}_{0,t_0}, \mathbf{y}_{0,t_0+\Delta}, \dots, \mathbf{y}_{0,t_0+K\Delta}$ } some initial encoding of the initial position \vec{r}_{t_0} . In particular, we define

 \mathbf{y}_{0,t_0} by assigning to each spatial pixel of the grid a value corresponding to the normalized distance

to the initial position of the particle eq.(5).

$$d = -\sqrt{\sum_{x \in \mathscr{D}} (\vec{r_{t_0}} - x)^2} \tag{5}$$

$$\mathbf{y}_{0,t_0} = \frac{d + |\min d|}{\max(d + |\min d|)} \tag{6}$$

while the other time steps of \mathbf{y}_0 are initialized as all-ones matrix of the same dimension as \mathcal{D} . The operator \mathscr{E} computes a latent embedding \mathbf{y} given velocity conditions \mathbf{u} and initial representation \mathbf{y}_0 , as introduced in eq.(3). And, the operator \mathscr{M} maps latent representation \mathbf{y} to the targeted Lagrangian drift \vec{r} . In other words, it maps a multi-dimensional tensor to a time series of locations in \mathscr{D} . The analytical expression of the operator \mathscr{M} for a given time step t grounds on the Hadamard product between the spatially-explicit encoding x of the space \mathscr{D} and \mathbf{y}_t field:

$$\mathscr{M} = \mathbf{x} \cdot \mathbf{y}_t \tag{7}$$

where $\mathbf{y}_t \in \mathbf{y}$, a sample of \mathbf{y} at a time step $t \in [t_0, \dots, t_{0+K\Delta}]$.

Regarding the operator \mathscr{E} , we consider the architecture sketched in Figure 1 and composed of:

1) a 2D convolutional layer increasing the number of channels from 3 (zonal and meridional components of **u** coupled to y_0) to 64, followed by a LeakyReLU activation function.

3) 2D convolutional layer decreasing the number of channels from 64 to 2, followed by 2D
 Softmax function.

Since our model is mainly based on 2D convolutional layers, we expect the resulting architecture 120 to capture relevant information at different space-time scales, and not only in a point-wise manner, 121 as it would be the case for the straightforward implementation of Fokker-Plank representation 122 eq.(3). Thus, our network can leverage non-local physical information explaining the particle's 123 motion and processes it to propagate the latent representation of particle's positions through time. 124 Interestingly, the proposed architecture easily generalizes to multi-source input data. Gridded 125 fields such as SSH fields with the same space-time resolution as the sea surface velocities convey 126 relevant information on sea surface dynamics. Stacking SSH and sea surface velocities, we may 127

¹²⁸ apply the same neural architecture, just increasing the number of channels of the input fields. The ¹²⁹ same applies for a prior on the diffusivity from the initial location of a particle in the field, that can ¹³⁰ be also included by stacking with the temporal evolution of the initial condition y_0 .

¹³¹ b. Learning scheme

We consider a supervised training of the proposed neural architecture according to the following
 two losses:

134 1. the Mean Square Error (MSE) between the reference and simulated trajectories for the *K*-step 135 simulation of N_T particles

$$\mathscr{L}_{MSE} = \frac{1}{N_T K} \sum_{i=0}^{N_T} \sum_{j=0}^K (\vec{r}_R(\vec{r}_{0,i}, j\Delta) - \vec{r}_S(\vec{r}_{0,i}, j\Delta))^2$$
(8)

- where \vec{r}_R and \vec{r}_S are the vector of positions of the reference and simulated trajectories respectively.
- ¹³⁸ 2. Liu index between the reference and simulated trajectories Liu and Weisberg (2011)

$$\mathscr{L}_{Liu} = \frac{1}{N_T} \sum_{i=1}^{N_T} \frac{\sum_{j=1}^K d_{i_j}}{\sum_{j=1}^K l_{i_j}}$$
(9)

139 where

$$d_{i_j} = \sqrt{(\vec{r}_R(\vec{r}_{0,i}, j\Delta) - \vec{r}_S(\vec{r}_{0,i}, j\Delta))^2}$$
(10)

is the Euclidean distance between the reference and the simulated trajectories number *i* at time step *j* and l_{ij} is the length of reference trajectory *i* between the initial position and the position at time step *j*.

¹⁴³ Overall, the training loss \mathscr{L} is a weighted sum: $\mathscr{L}_{Liu} = \alpha \cdot \mathscr{L}_{MSE} + \beta \cdot \mathscr{L}_{Liu}$. From cross-validaton ¹⁴⁴ experiments, we set α and β to 0.2 and 0.8. Using Pytorch², our learning setup relies on Adam ¹⁴⁵ optimizer with a learning rate of 5e-3 over 750 epochs.

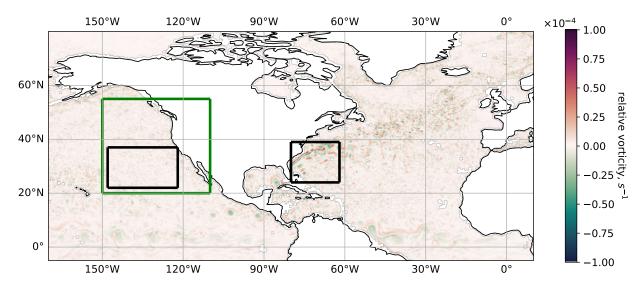


FIG. 2: **Study cases delineation:** Relative vorticity of North East Pacific and North Atlantic oceans from E1 simulation of 01/10/2015. The two black boxes indicate the North East Pacific and Gulf Stream case study regions for benchmarks B1 and B2. The green box defines the North East Pacific region of study for benchmark B3.

146 **4. Experimental workflow**

Section 4.a details the two case-study regions considered because of their contrasting turbulent activity: the Gulf Stream and the North-East Pacific region, see Figure 2. We describe the different datasets used in our experiments in section 4.b, see Table 1, and the metrics used to evaluate performance in section 4.c. In section 4.d we present the benchmarked deep learning models. We perform three different experiments: two relying on numerical simulation datasets such that the full sea surface velocity field is known, and a last experiment dealing with real drifters in the sea surface. These three benchmarks are explained in section 4.e.

154 a. Case-study Regions

The Gulf Stream is a Western boundary current system characterized by a fast flowing jet that originates in the Gulf of Mexico and flows into the North Atlantic Gula et al. (2015); Dewar and Bane (1989), becoming a part of it's anticyclonic subptropical gyre Talley (2011). Surface velocity can exceed $2 m \cdot s^{-1}$ and the current is characterized by high eddy variability. Exhibiting strong velocities for hundreds of kilometers, the Gulf Stream transports warm saline water from lower latitudes north-eastward. The Gulf Stream plays a crucial role in redistributing heat and

²DriftNet code is available at https://github.com/CIA-Oceanix/DriftNet

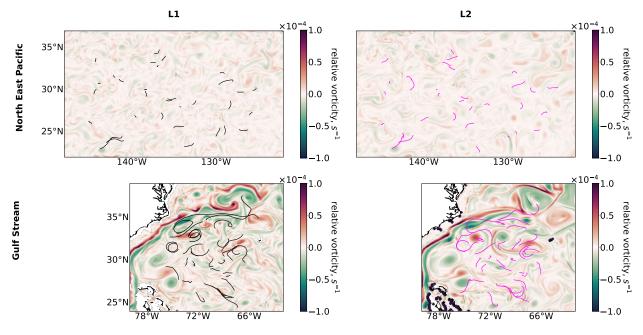


FIG. 3: **Examples of trajectories:** Trajectories from dataset L1 and dataset L2 superimposed respectively to the E1 and E2 relative vorticity fields of 2015/01/01.

¹⁶¹ influencing climate patterns and the surrounding marine ecosystem Gula et al. (2015), Wills et al. ¹⁶² (2016).

The North East Pacific is a vast oceanic region extending from the western coast of North 163 America to the central Pacific. It is influenced by various ocean currents, including the California 164 Current and North Pacific Current. The California Current System (CCS) is an eastern boundary 165 of the slow (0.1 $m \cdot s^{-1}$) eastward North Pacific Current. It is a cold, nutrient-rich current that 166 flows southward along the Western coast of North America Checkley and Barth (2009); Auad 167 et al. (2011), impacting marine ecosystems and fisheries. The CCS is an upwelling region due to 168 Ekman transport, spining up eddies westward offshore. It has a mean surface velocity of 0.4 - 0.8169 $m \cdot s^{-1}$. Due to the baroclinic instability of the coastal upwelling current, the CCS contains high 170 mesoscale eddy activity, associated with the highly variable sea-surface height Talley (2011). 171

172 b. Datasets

Our study involves three different Eulerian datasets used as input data for the benchmarked models: TABLE 1: Summary description of the Eulerian and Lagrangian datasets used in the current study: *Source* makes reference to the used numerical or satellite product, *Variable* indicates the physical quantity of interest, *Period* the studied years. The spatial and temporal resolutions of each product are also indicated. SSC - sea surface currents. SSH - sea surface height.

| Name | Source | Variable | Period | Spatial resolution | Temporal resolution |
|------------|---|-------------|-------------|--------------------|---------------------|
| Eulerian | | | | | |
| E1 | Nature Run | SSC and SSH | 2015 | 1/12° | 1 day |
| E2 | OSSE-based assimilated free run | SSC | 2015 | 1/12° | 1 day |
| E3 | Operational assimilated reanalysis GLORYS12 | SSC | 1992 - 2020 | 1/12° | 1 day |
| E3 | DUACS | SSH | 1992 - 2020 | 1/4° | 1 day |
| Lagrangian | | | | | |
| L1 | Ocean Parcels simulation on E1 SSC | Position | 2015 | - | 6 hours |
| L2 | Ocean Parcels simulation on E2 SSC | Position | 2015 | - | 6 hours |
| L3 | CMEMS drifters | Position | 1992 - 2020 | - | 6 hours |
| L4 | Ocean Parcels simulation on E3 SSC | Position | 1992 - 2020 | - | 6 hours |

Eulerian dataset E1: This Eulerian dataset contains the sea surface current (SSC) velocity and sea surface height (SSH) fields. Both fields are obtained from a high-resolution free simulation of the NEMO ocean model without any data assimilation Benkiran et al. (2021b). Those are regularly-gridded products with a horizontal spatial resolution of 1/12° and a daily time resolution. This study involves the entire year of 2015.

Eulerian dataset E2 This dataset contains the SSC fields from a data assimilated run, which dynamically reconstructs the ocean state using pseudo observations from E1 which mimic the current observational network (satellite altimetry tracks). Those fields are at the same 1/12° and daily space-time resolution as the E1 dataset. As in the previous E1 dataset, we equivalently use the complete 2015 year.

 Eulerian Real-world dataset E3: this real-world dataset combines the SSC from the operational ocean reanalysis GLORYS12 Lellouche et al. (2021) and the optimally-interpolated altimetry-derived SSH product DUACS Pujol et al. (2016). The GLORYS12 velocity fields are provided on the regular grid with spatial resolution of 1/12° and temporal resolution of 1 day. We re-interpolate the SSH fields on the same 1/12° regular grid at daily temporal resolution. For each individual trajectory, the considered spatial domain of the Eulerian conditional fields is equal to, $4^{\circ} \times 4^{\circ}$ window for the North East Pacific and $10^{\circ} \times 10^{\circ}$ for the Gulf Stream. The size of the domains corresponds to the furthest displacement from a given particle's deployment location in each case study region.

¹⁹⁵ Our benchmarks involve four different Lagrangian datasets:

Lagrangian Dataset L1: this dataset is composed of 9-day trajectories of virtual particles advected by the sea surface velocities from dataset E1 using Ocean Parcels, a state-of-the-art tool for model-based Lagrangian drift simulation Lange and van Sebille (2017). Around 20 particles were randomly seeded every day across the domain and the studied period, amounting to a total of 7900 particles.

Lagrangian Dataset L2: this dataset contains 9-day trajectories of virtual particles advected by the SSC of the E2 dataset with Ocean Parcels. It contains 7900 particles deployed at the exact same locations and times as in the Lagrangian Dataset L1 described above, see Figure 3.

• Lagrangian Dataset L3 This dataset contains trajectories from CMEMS drifters Etienne 204 et al. (2023) in the North East Pacific region, from 1992 to 2020. Those drifters are a part 205 of the Surface Velocity Program (SVP) and are built of 1-m long floating buoy attached to a 206 "drogue" deployed at 15 meters depth in order to reduce the windage slip Lumpkin et al. 207 (2017). Drifters positions are subject to a quality control and editing procedures before 208 being operational. Subsequently, trajectory positions undergo regular reinterpolation using 209 the Kriging technique at 6-hour intervals Etienne et al. (2023). For this study, we refer to 210 drogued-only drifters which are representative of the ocean currents at 15 meters depth and 211 are widely used in various application domains Lumpkin et al. (2012); Koszalka et al. (2011); 212 Lumpkin and Flament (2013); Kaplan et al. (2005); Lumpkin and Garzoli (2011). 213

This dataset contains 12.785 9-day trajectories in the North East Pacific case-study region, green box in Figure 2. These trajectories are obtained by dividing the whole drifter trajectories of the region in 9-day long non-overlapping segments.

Lagrangian Dataset L4: this dataset contains 9-day trajectories of virtual particles advected by the velocity fields from E3 with Ocean Parcels. We use the same initial deployment position and time of the trajectories as in dataset L3.

12

- 220 c. Performance metrics
- As evaluation metrics, we consider
- the mean Euclidean distance at the last time step (9-th day) in kilometers, that we denote D:

$$D = \frac{1}{N_T} \cdot \sum_{i=0}^{N_T} d_{i_{9\Delta}} \tag{11}$$

- with N_T the number of trajectories and $d_{i_{9\Lambda}}$ defined in eq.(10) with j = 9 days.
- the Mean Liu index \mathscr{L}_{Liu} without units, see eq.(9).

• the Mean absolute error between Lagrangian Time Scales $\Delta \mathscr{T}$ Krauß and Böning (1987), in days:

$$\Delta \mathscr{T} = \frac{1}{N_T} \cdot \sum_{i=0}^{N_T} |\mathscr{T}_{R_i} - \mathscr{T}_{S_i}|$$
(12)

where \mathscr{T}_{R_i} and \mathscr{T}_{S_i} are respectively the Lagrangian time of the reference and simulated i-th trajectory defined as:

$$\mathscr{T} = \int_{t_0}^{t_0+9\Delta} R_{\vec{v}}(\tau) d\tau \tag{13}$$

where $R_{\vec{v}}(\tau) = \frac{1}{9\cdot\Delta} \cdot \sum_{t=0}^{9} \vec{v}(t\Delta + \tau)\vec{v}(t\Delta)$ is the autocorrelation function of the Lagrangian velocity of a given particle.

These three metrics are computed between the reference and generated trajectories and averaged over the whole ensemble of studied trajectories.

233 d. Benchmarked deep learning models

To evaluate the performance of DriftNet, we compare it to the following CNN and LSTM baselines inspired by Zheng et al. (2022); Ma et al. (2019):

• Convolutional Neural Network (CNN): a 2D convolutional block varying the number of channels from 27 (**u** and **y**₀ concatenated along the time dimension) to $8 \rightarrow 16 \rightarrow 32 \rightarrow 35$. Each convolution layer has a kernel of size 5 and is followed by a LeakyReLU activation function
with a slope of 0.2 for negative inputs. The output of this convolutional block is introduced
by a reshape, where the two spatial dimensions of initial 3d matrix are flattened together,
and the output is passed to a fully connected layer with 256 and 128 neurons decreasing the
mentioned spatial dimension to 2.

Long Short-Term Memory (LSTM): a 5-layer LSTM block with hidden size 96, followed by
 a ReLU activation function, then two fully connected layers with a ReLU in between. Each
 dense layer contains 864, and 128 neurons respectively, reducing the latent space to 2.35.
 This output is then reshaped so to contain the spatial dimension 2 and temporal one 35.

We also explore different configurations of DriftNet. In order to investigate the impact of each
component of the model on the evaluation metrics, we modify its inner architecture, see section
3. a and Figure 1, and assess the performance of the following three architectures:

• DriftNet without the ConvLSTM block in the encoding operator \mathscr{E} ;

• DriftNet without the CNN block in the encoding operator \mathscr{E} ;

a DriftNet-Unet architecture, referred to as DriftNet_U: in this architecture, we replace the CNN block in the encoding operator & by a U-net block. The latter is composed of three 2d Conv-MaxPool-ReLU layers with kernel size 3 and channels evolving from 27 to 256 and three 2d ConvTranspose-Upsample-ReLU layers with kernel size 3 and channels evolving from 256 to 27.

257 e. Benchmarks

This section presents the experimental setups that we employ to assess the performance of Drift-Net in both virtual and real-case scenarios.

Benchmark B1 This benchmark B1 aims to assess the reliability and accuracy of learningbased schemes in reproducing Lagrangian drift trajectories given fully-known underlying dynamics. This benchmark uses the Eulerian velocity field extracted from the dataset E1 and the trajectories from the Lagrangian Dataset L1. The resulting dataset is randomly splitted into train (80%), validation (10%) and test (10%) sets. DriftNet is fed with E1 velocity fields and trained to reproduce reference trajectories from the L1 dataset. For benchmarking purposes, we consider the
 CNN and LSTM baselines trained following the same strategy as DriftNet.

Benchmark B2 This benchmark aims to assess from simulation data the ability to predict accurately Lagrangian drift trajectories when the sea surface velocities are imperfectly known. We use E2 velocity fields and L1 trajectories as reference. Similarly to Benchmark B1, we randomly split the resulting dataset into train (80%) validation (10%) and test (10%) datasets. For benchmarking purposes, we consider the state-of-the-art model-based method corresponding to trajectory dataset L2 as well as the CNN and LSTM baselines trained following the same strategy as DriftNet.

Benchmark B2 also assesses the ability of DriftNet to exploit multi-source geophysical data.
Here, we complement the data with the Sea Surface Height (SSH) from Dataset E1. In this configuration, Driftnet is fed with E2 velocity fields and E1 SSH fields to reproduce L1 trajectories.

Benchmark B3 This benchmark addresses a real-case scenario with real drifters' trajectories
and operational ocean reanalyses. We use E3 velocity and SSH fields and real trajectories from L3
dataset as reference. Similarly to Benchmark B1, we randomly split the resulting datasetinto train
(70%) validation (10%) and test (20%) datasets.

For benchmarking purposes, we consider the state-of-the-art model-based method corresponding to trajectory dataset L4 as well as the CNN and LSTM baselines trained following the same strategy as DriftNet. This benchmark assesses a DriftNet using solely E3 velocity fields and a DriftNet using jointly E3 velocity and SSH fields.

284 **5. Results**

This section reports our numerical experiments for the three benchmarks introduced in the previous section, namely benchmark B1 (section 5.a), benchmark B2 (section 5.b) and benchmark B3 (section 5.c).

288 a. Results for Benchmark B1

DriftNet presents the best performance for all metrics and significantly outperforms the CNN and LSTM baselines, see Table 2. For the North East Pacific, the separation distance of 5.3km after 9 days is of around one order of magnitude smaller than the baseline CNN and LSTM models. Similar performances are noted for Liu index, 0.06, and the error between Lagrangian time scales, TABLE 2: **Performance of DriftNet for Benchmark B1**: we report the performance metrics for DriftNet and classical learning-based approaches for benchmark B1 in the two study regions: North East Pacific and Gulf Stream. The evaluation metrics are the last time step mean separation distance (D), mean Liu index (\mathscr{L}_{Liu}) and mean absolute error between Lagrangian time scales ($\Delta \mathscr{T}$). Bold indicates the best performance. We refer the reader to section 4.d for the details of the benchmarked architectures.

| | | North East Pacific | | | Gulf Stream | |
|----------|-------|---------------------|-----------------------------|--------|---------------------|-----------------------------|
| Method | D, km | \mathscr{L}_{Liu} | $\Delta \mathscr{T}$, days | D, km | \mathscr{L}_{Liu} | $\Delta \mathscr{T}$, days |
| DriftNet | 5.3 | 0.06 | 0.14 | 91.1 | 0.26 | 1.17 |
| CNN | 43 | 0.5 | 1.46 | 151.85 | 0.63 | 4.03 |
| LSTM | 30.6 | 0.4 | 3.36 | 188 | 0.77 | 4.42 |

0.14. For the Gulf Stream, the overall accuracy is lower (separation distance after 9 days of
 91.1km, Liu index 0.26 and Lagrangian time scale error 1.17), but still DriftNet outperforms the
 baselines. These experiments support the proposed Eulerian Fokker-Plank-inspired architecture.

DriftNet simulation error is larger for the Gulf Stream region. This is consistent with the resolution error in encoding initial positions, as evidenced in Callies et al. (2021). Here, Lagrangian trajectories simulated with an error corresponding to the resolution of the grid (*i.e.*, 1/12°) leads to a separation distance after 9 days of 20km (resp. 94km) for the North East Pacific region (resp. the Gulf Stream region). The larger sea surface velocities and sharper associated spatial gradients in the Gulf Stream region explains the larger separation distance after 9 days.

Impact of DriftNet components we compare DriftNet in it's original configuration to three variations presented in section 4.d namely a configuration combining two commonly used
 U-Net models separated by one ConvLSTM block, a second one containing the ConvLSTM block only, and finally one composed of 2D convolutional layers only.

Removing the CNN or LSTM blocks from the DriftNet architecture impacts the simulation performance, see Table 3. The separation distance increases from 5.3km to 42.1km (resp. 36.2km) for the North East Pacific region when we remove the LSTM (resp. CNN) block. Similarly, the U-Net version of the DriftNet does not lead to a better simulation performance. This likely relates to some overfitting in our training schemes due to the greater complexity of this UNet configuration. Same qualitative results are found in the Gulf Stream region. TABLE 3: **Ablation study of DriftNet**: we compare the metrics of different configurations of DriftNet for benchmark B1: namely, the reference DriftNet, DriftNet_U with a U-net block instead of CNN, a DriftNet without the CNN block and DriftNet without ConvLSTM. The evaluation metrics are the last time step mean separation distance (D), mean Liu index (\mathscr{L}_{Liu}) and mean absolute error between Lagrangian time scales ($\Delta \mathcal{T}$). Bold indicates best performance.

| | North East Pacific | | Gulf Stream | | | |
|---------------------------|--------------------|---------------------|-----------------------------|-------|---------------------|-----------------------------|
| Method | D, km | \mathscr{L}_{Liu} | $\Delta \mathscr{T}$, days | D, km | \mathscr{L}_{Liu} | $\Delta \mathscr{T}$, days |
| DriftNet | 5.3 | 0.06 | 0.14 | 91.1 | 0.26 | 1.17 |
| $DriftNet_U$ | 16.1 | 0.21 | 1.79 | 96 | 0.32 | 0.9 |
| DriftNet without CNN | 36.2 | 0.39 | 0.32 | 163 | 0.68 | 1.7 |
| DriftNet without ConvLSTM | 42.1 | 0.37 | 1.45 | 177 | 0.73 | 2.84 |

TABLE 4: **Impact of spatial resolution on DriftNet performance** Performance of DrifNet in function of the spatial resolution of the input Eulerian velocity field for benchmark B1 in both study regions: North East Pacific and Gulf Stream. Each line corresponds to a different spatial resolution of the input E1 field. The evaluation metrics are the last time step mean separation distance (*D*), mean Liu index (\mathscr{L}_{Liu}) and mean absolute error between Lagrangian time scales ($\Delta \mathcal{T}$). Bold indicates best performance.

| | North East Pacific | | | | | |
|--------------------------------|--------------------|---------------------|-----------------------------|-------|---------------------|-----------------------------|
| Resolution | D, km | \mathscr{L}_{Liu} | $\Delta \mathscr{T}$, days | D, km | \mathscr{L}_{Liu} | $\Delta \mathscr{T}$, days |
| $1/12^\circ \times 1/12^\circ$ | 5.3 | 0.06 | 0.14 | 91.1 | 0.26 | 1.17 |
| $1/6^\circ \times 1/6^\circ$ | 8.7 | 0.15 | 0.17 | 102.3 | 0.35 | 1.23 |
| $1/3^\circ \times 1/3^\circ$ | 17.9 | 0.27 | 0.28 | 109.4 | 0.47 | 0.91 |
| $1/2^\circ \times 1/2^\circ$ | 28.2 | 0.40 | 0.99 | 115.9 | 0.46 | 1.05 |

Impact of the resolution of the conditioning velocity fields. Coarsening the resolution of the conditioning fields leads to degrading the performance, see Table 4. For both regions, the impact is more significant in the mean separation distance and the Liu index, while Lagrangian time scale estimation does not seem to be impacted by the degradation in the underlying resolution. Resolution is thus an important characteristic of the input fields.

317 b. Results for Benchmark B2

Table 5 illustrates the performance of the simulation of Lagrangian trajectories using degraded velocity fields instead of the true velocity fields. Similarly to Benchmark B1, we compare DriftNet to CNN and LSTM baselines. Here we also benchmark DriftNet with respect to the Lagragian simulations with Ocean Parcels Lange and van Sebille (2017). TABLE 5: **Performance metrics for Benchmark B2 experimental framework**. We report the performance metrics for DriftNet and baseline models, all supplied with velocity fields from E2 and trained to generate trajectories from reference Dataset L1 in the two study regions: North East Pacific and Gulf Stream. The evaluation metrics are the last time step mean separation distance (D), mean Liu index (\mathscr{L}_{Liu}) and mean absolute error between Lagrangian time scales $(\Delta \mathcal{T})$. Bold indicates the best performance.

| | | North East Pacific | | | Gulf Stream | |
|---------------|-------|---------------------|-----------------------------|-------|---------------------|-----------------------------|
| Method | D, km | \mathscr{L}_{Liu} | $\Delta \mathscr{T}$, days | D, km | \mathscr{L}_{Liu} | $\Delta \mathscr{T}$, days |
| Ocean Parcels | 53.6 | 0.87 | 0.1 | 168.3 | 0.75 | 0.04 |
| DriftNet | 45.4 | 0.7 | 1.96 | 154.6 | 0.63 | 1.82 |
| CNN | 51.7 | 0.72 | 2.12 | 184.1 | 0.67 | 2.48 |
| LSTM | 47.9 | 0.69 | 4.35 | 163.2 | 0.67 | 2.1 |

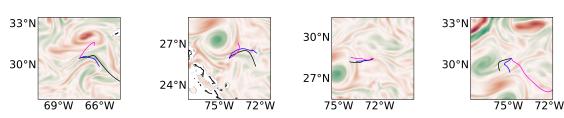
³²² DriftNet presents smaller D 45.4 km (154.6 km) and $\Delta \mathscr{T}$ than the other learning-based models, ³²³ and smaller D, \mathscr{L}_{Liu} than Ocean Parcels, thus consistently outperforming the baseline approaches. ³²⁴ The \mathscr{L}_{Liu} for the North East Pacific region is of 0.7 and is smaller than the most baseline ap-³²⁵ proaches, except the LSTM model (0.69) slightly outperforming the proposed method. While in ³²⁶ the Gulf Stream the \mathscr{L}_{Liu} (0.63) is smaller than all the other approaches. The Lagrangian time ³²⁷ scale error is larger for the proposed method than for the baseline Ocean Parcels.

Impact of auxiliary variables Table 6 assesses how the availability of the SSH fields could 328 improve the simulation of Lagrangian drift trajectories. Whereas Lagrangian model eq.(1) solely 329 depends on the sea surface velocities, deep learning schemes can easily extend to multiple condi-330 tioning fields. Among the observed satellite-derived tracers on the sea surface, the SSH explicitly 331 seems appealing as it informs the geostrophic component of sea surface currents Taqi et al. (2019); 332 Ballarotta et al. (2022). In an idealized setting, we evaluate the potential added value of the true 333 SSH fields provided as inputs to DrifNet either in place of E2 velocity fields or to complement 334 them, see Table 6. 335

These results emphasize the synergistic potential of SSH observations and E2 velocity fields compared with using only one of these two input data. In the North East Pacific region, D is reduced by over 55%, \mathcal{L}_{Liu} by over 60% and $\Delta \mathcal{T}$ by over 45%. Similarly in the Gulf Stream, we report a relative gain greater than 25% for D, 30% for \mathcal{L}_{Liu} and 20% for $\Delta \mathcal{T}$. These results are in agreement with the ability of observation-based SSH products to capture geostrophic dynamics Ballarotta et al. (2022), while data-assimilation-based velocity fields can reveal the

38°N ×10⁻⁴ 1.00 36°N 0.75 0.50 34°N elative vorticity 0.25 32°N 0.00 -0.25 30°N S -0.50 28°N -0.75 26°N -1.00 75 72.5°W 70°W 67.5°W 65°W 62.5°W L1 L2 Proposed method (b) 36°N 33°N 27°N 33°N 30°N 24°N 72°W 69°W 70°W67.5°W 75°W 72°W 72.5°W70°W

(a)



33°N

30°N

FIG. 4: **Trajectories for Benchmark B2 in the Gulf Stream** Lagrangian trajectories from Dataset L2 are depicted in magenta, trajectories simulated with DriftNet conditioned with SSC from E2 and SSH from E1 in blue, and trajectories from Dataset L1 in black. For better visual appreciation panel a) shows 16 randomly picked trajectories for the whole region while b) shows 8 random trajectories zoomed. All superimposed to the mean relative vorticity field of E1.

³⁴² ageostrophic sea surface dynamics. The latter are expected to be significant for horizontal scales

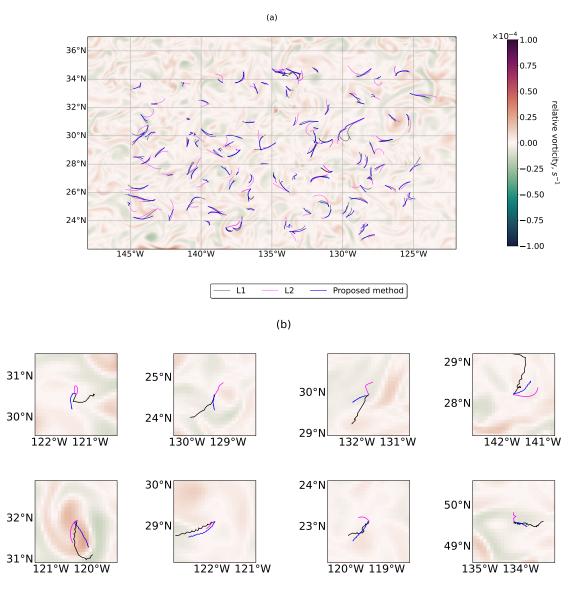


FIG. 5: **Trajectories for Benchmark B2 in the North East Pacific** Lagrangian trajectories from Dataset L2 are depicted in magenta, trajectories simulated with DriftNet conditioned with SSC from E2 and SSH from E1 in blue, and trajectories from Dataset L1 in black. a) shows 128 randomly picked trajectories for the whole region while b) shows 8 random trajectories zoomed. All superimposed to the mean relative vorticity field of E1.

- ³⁴³ below a few hundreds of kilometers, especially in Western Boundary currents such as the Gulf
- ³⁴⁴ Stream Gula et al. (2015).
- ³⁴⁵ For both regions the trajectories are visualised at the Figure 4 and Figure 5 which show that
- ³⁴⁶ DriftNet generates trajectories closer to the ground truth from L1 than the baseline L2.

TABLE 6: Synergistic use of SSH observations and data-assimilation-based velocity fields in Benchmark B2. We beenhmark DriftNet schemes using as inputs data-assimilation-based velocity fields from dataset E2 and idealized perfectly-observed Sea Surface Height (SSH) fields (i.e., SSH fields from dataset E1). We illustrate performance in the two study regions: North East Pacific and Gulf Stream. The evaluation metrics are the last time step mean separation distance (D), mean Liu index (\mathscr{L}_{Liu}) and mean absolute error between Lagrangian time scales $(\Delta \mathcal{T})$. Bold indicates the best performance.

| North East Pacific | | | | Gulf Stream | | |
|----------------------|-------|---------------------|-----------------------------|-------------|---------------------|-----------------------------|
| Method(Variable) | D, km | \mathscr{L}_{Liu} | $\Delta \mathscr{T}$, days | D, km | \mathscr{L}_{Liu} | $\Delta \mathscr{T}$, days |
| DriftNet (U, V) | 45.4 | 0.71 | 1.96 | 157 | 0.73 | 1.84 |
| DriftNet (SSH) | 31.2 | 0.32 | 1.32 | 160.3 | 0.7 | 1.41 |
| DriftNet (U, V, SSH) | 22.2 | 0.29 | 0.73 | 127 | 0.52 | 1.44 |

TABLE 7: **Performance metrics for Benchmark B3**. Performance of different Lagrangian simulation schemes for Benchmark B3 which involves real data. For each scheme, we detail the considered input data: namely the velocity fields U and V from the GLORYS12 reanalysis Lellouche et al. (2018) possibly complemented by satellite-derived optimally-interpolated SSH fields Pujol et al. (2016). We report the performance metrics in the two study regions: North East Pacific and Gulf Stream. The evaluation metrics are the last time step mean separation distance (*D*), mean Liu index (\mathscr{L}_{Liu}) and mean absolute error between Lagrangian time scales ($\Delta \mathscr{T}$). Bold indicates the best performance.

| | | North East Pacific | |
|----------------------|-------|---------------------|-----------------------------|
| Method(Variable) | D, km | \mathscr{L}_{Liu} | $\Delta \mathscr{T}$, days |
| Ocean Parcels (U, V) | 73.77 | 0.65 | 2.2 |
| DriftNet (U, V) | 62.9 | 0.55 | 0.71 |
| CNN (U, V) | 68.64 | 0.57 | 0.32 |
| LSTM (U, V) | 64.3 | 0.55 | 2.1 |
| DriftNet (U, V, SSH) | 60.2 | 0.52 | 0.04 |

347 c. Results for Benchmark B3

In this real case situation, DriftNet outperforms the classical advection method, see Table 7 and Figure 6. Compared to the model-based baseline, the mean separation distance of 62.9km is reduced by around 15%, the Liu index of 0.55 by 15%. Unlike previous B2 experiment, the Lagrangian time scale error of 0.71 is significantly reduced. As in benchmark B2, we observe a significant impact of the observed SSH fields in the quality of the simulation of the Lagrangian trajectories. The combination of GLORYS12 velocities and satellite-derived SSH fields leads to a reduction of the mean separation distance by over 4% compared to the baseline DriftNet and ³⁵⁵ by over 18% compared to the baseline model-based advection method. The Liu index is also ³⁵⁶ reduced by more than 5% compared to the DriftNet baseline and by over 20% compared to the ³⁵⁷ baseline advection method. The Lagrangian time scale error is significantly reduced, by over ³⁵⁸ 94% compared to the DriftNet baseline and by over 98% compared to the baseline model-based ³⁵⁹ approach.

6. Conclusions and Discussion

In this study, we presented a novel deep learning framework, called DriftNet, for the conditional simulation of Lagrangian drift trajectories on the sea surface. We drew inspiration from the Fokker-Planck equation to explore a spatially-explicit Eulerian latent representation of the trajectories in the proposed neural architecture. We evaluate DriftNet on three different benchmarks using synthetic and real-world datasets. Our experiments support the relevance of DriftNet to advance Lagrangian drift simulations on the sea surface and better exploit available reanalysis and observation datasets.

DriftNet consistently demonstrated a better performance than state-of-the-art model-based and 368 learning- based approaches, with respect to the following Lagrangian metrics: mean separation 369 distance, Liu index and Lagrangian time scale error between the ground-truth trajectories and 370 the simulated ones. When DriftNet is provided with fully known velocity fields from Nature 371 Run simulation (Benchmark B1), it reduces the overall error by more than 80% compared to the 372 state-of-the-art learning-based approaches. Moreover, when DriftNet is provided with degraded 373 velocity fields from OSSE-based assimilated simulation (Benchmark B2), it reduces the overall 374 error by over 15% compared to conventional point-wise schemes. These results are consistent for 375 the two case-study regions, even if they are characterized by notably different dynamical regimes. 376 Interestingly, we draw similar conclusions between synthetic and real datasets. 377

The performance of DriftNet exhibits variabilities across the two different regions. It likely underscores the importance of region-specific adaptations in trajectory simulation models. As such, the deployment of DriftNet on a global scale may require retraining the model to accommodate the diverse dynamics in various oceanic regions Miao et al. (2023). While we expect the proposed neural architecture to be generic, fine-tuning its parameters to align with the characteristics of a given region seems crucial for the relevance of the simulations. This approach allows for the incor-

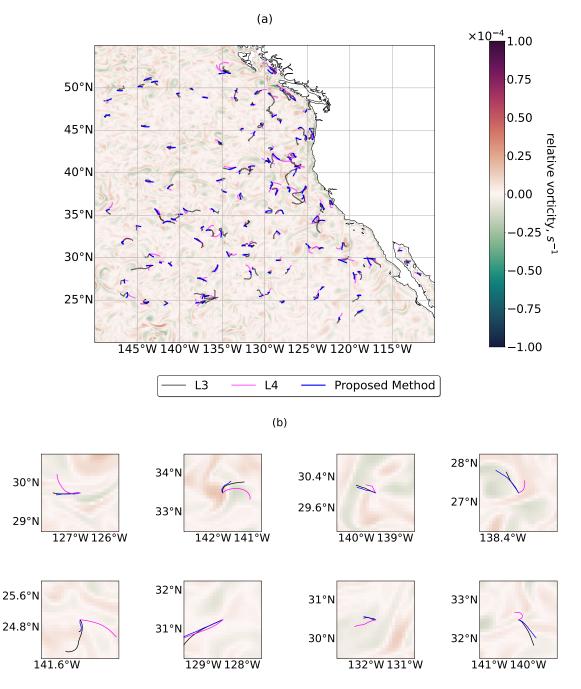


FIG. 6: **Examples of simulated trajectories for Benchmark B3**: we depict real drifters trajectories in black (L3), trajectories simulated with Ocean Parcels using GLORYS12 velocity fields in magenta (L4) and trajectories simulated with DriftNet using both GLORYS12 velocity fields and satellite-derived optimally-interpolated SSH fields in blue. Panel (a) illustrates trajectories from the whole region. Panel (b) zoom on a subset of randomly-selected trajectories. All superimposed to the mean relative vorticity of the GLORYS12 velocity fields.

³⁸⁴ poration of region-specific features, thereby enhancing the model's predictive capabilities across ³⁸⁵ diverse geographical regions. Furthermore, leveraging transfer learning techniques to capitalize ³⁸⁶ on the knowledge gained from training in one region to inform model adjustments in others holds ³⁸⁷ promising avenue. By iteratively refining DriftNet through region-specific training and fine-tuning ³⁸⁸ iterations, we hope to develop a robust trajectory simulation tool capable of capturing the intrica-³⁸⁹ cies of oceanic dynamics on a global scale.

Our benchmarks highlight the relevance of the SSH fields to improve the prediction of La-390 grangian drifts on the sea surface both in synthetic and real case-studies, *i.e.* Benchmarks B2 391 and B3. We report a significant improvement for all the considered metrics when we comple-392 ment reanalysis velocity fields with SSH fields. The SSH informs the geostrophic component of 393 the sea surface currents, which is important for the two case-study regions for horizontal scales 394 above 100km Checkley and Barth (2009); Thomas and Joyce (2010); Johns et al. (1989). As ocean 395 reanalysis datasets can usually retrieve sea surface currents for horizontal scales above a few hun-396 dred of kilometers Benkiran et al. (2021a); Lellouche et al. (2021), the learning schemes likely 397 benefit from the SSH fields to recover a more robust representation of the sea surface dynamics 398 and improve the simulation of Lagrangian drift on the sea surface. The advent of wide-swath 399 satellite altimeters Benkiran et al. (2021b); Tchonang et al. (2021), possibly combined with neural 400 mapping schemes Martin et al. (2023); Beauchamp et al. (2022); Fablet et al. (2023), will lead 401 to a better reconstruction of satellite-derived SSH fields, which could in turn result in improved 402 learning-based Lagrangian simulations for real drifters on the sea surface. 403

Beyond the exploraton of satellite-derived SSH fields, the use of additional geophysical variables 404 to enhance trajectory generation offers another interesting approach to improve the simulation 405 performance. Future studies could investigate other variables such as Sea Surface Temperature 406 Ciani et al. (2020), Ocean Color Yang et al. (2015); Liu et al. (2017), Winds Cucco et al. (2016); 407 Solanlki et al. (2001) or Waves Tang et al. (2007) to refine trajectory simulations and gain deeper 408 insights into oceanic processes. By leveraging these variables, the proposed method could not only 409 improve trajectory accuracy but also facilitate comprehensive analysis of the underlying ocean 410 dynamics. 411

Inspired by established initiatives such as WeatherBench Rasp et al. (2020) and OceanBench Johnson et al. (2024), we propose a new benchmark for a standardized assessing and comparing Lagrangian trajectory simulation models https://github.com/CIA-Oceanix/DriftNet. Through proposed datasets and evaluation metrics, this framework seeks to foster collaborative frameworks involving ocean scientists and ML practitioners. In this context, future work could explore new evaluation metrics and extend the proposed benchmarks to a broader array of oceanic regions.

From a methodological point of view, it seems appealing to extend the DriftNet to a probabilistic 418 framework with a view to sampling ensembles of realistic drift trajectories. Conditional Genera-419 tive Adversarial Networks (GAN) Roy et al. (2022) naturally arise among the promising solutions. 420 Other generative models such as diffusion models Tashiro et al. (2021) could also be explored. Re-421 garding real-time operational applications, such as search and rescue operations, or iceberg drifts, 422 such generative schemes would also naturally apply to the short-term forecasting of Lagrangian 423 trajectories on the sea surface using sea surface conditions issued from short-term forecasts. This 424 research direction would likely benefit from the development of neural ocean forecasts Wang et al. 425 (2024); Xiong et al. (2023) to advance model-based operational forecasts Drévillon et al. (2008); 426 Benkiran et al. (2024). 427

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⁴³⁷ Data availability statement. The data used in this study, including ocean currents and sea surface ⁴³⁸ height are openly accessible through the Copernicus Marine Environment Monitoring Service ⁴³⁹ (CMEMS). The data from the B1 and B2 benchmarks are subject to access restriction, one should ⁴⁴⁰ refer to Mercator Ocean International in order to claim the access rights. Additionally, the code ⁴⁴¹ implemented for the evaluation of the methods discussed in this article is available as an open-⁴⁴² source project on GitHub: https://github.com/CIA-Oceanix/DriftNet.

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