Regional Ocean Forecasting with Hierarchical Graph Neural Networks

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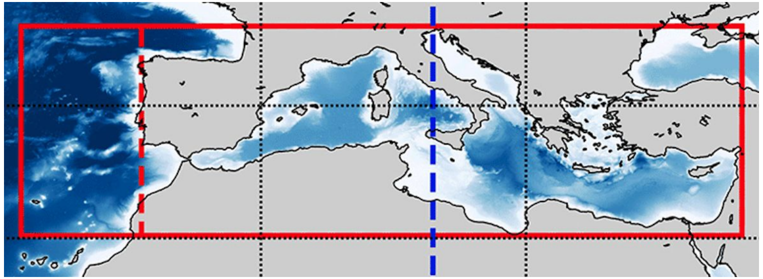
Standard Numerical Mediterranean Forecasting

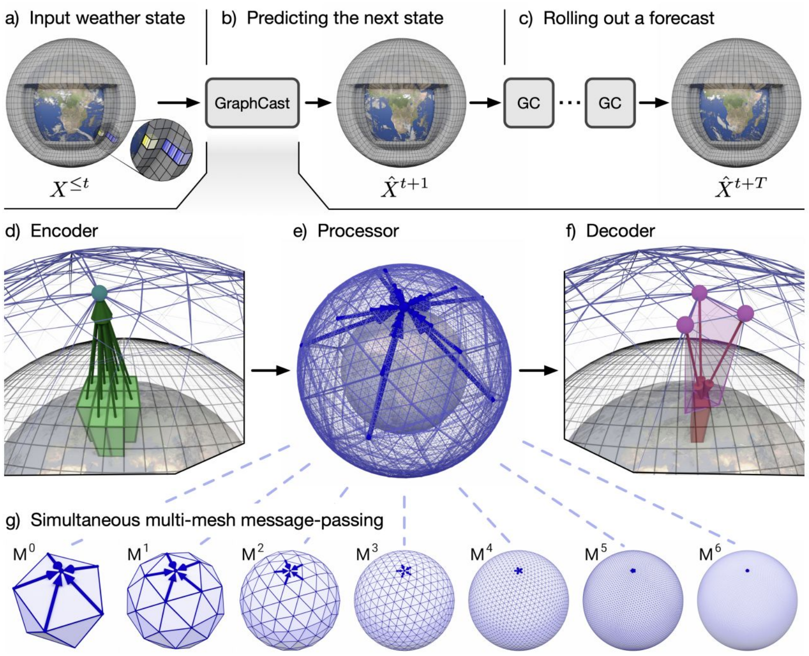
- Uses Nucleus for European Modelling of the Ocean (NEMO) to simulate physical ocean processes such as currents, temperature, and salinity numerically.
- Incorporates observational data (in situ measurements, remotely sensed data) into models using variational ocean data assimilation (OceanVar).
- Interpolated simulation grid based on General Bathymetric Chart of the Oceans (GEBCO).
- Operates on high-resolution 1/24° grid with 141 vertical levels.
- Open boundaries at Gibraltar and Dardanelles.
- River runoff, e.g. Rhône, Po, and the Nile.
- Forced with surface atmospheric quantities.



The Mediterranean Forecasting System–Part 1: Evolution and performance. Ocean Science (2023)

Proposed Method

- Train a graph neural network (GNN) to autoregressively predict next simulation step. Meaning, predicted state is used as input to predict the following state after that.
- Produces a cumulative error, and smoothening as time goes on.
- However, for ocean forecasting the method is promising: reasonable amount of rollout steps needed.
- Large advantage in terms of prediction speed vs numerical simulations.



Remi Lam et al., Learning skillful medium-range global weather forecasting. Science (2023)

Mediterranean Sea Physics Dataset

Variables

- Covers the epipelagic zone with every other simulated depth (18 total) down to 200 meters.
- 75 variables in total (18×4 + 3): potential temperature, salinity, meridional and zonal velocity + single level SSH, bottom temperature and mixed layer depth.

Training Set

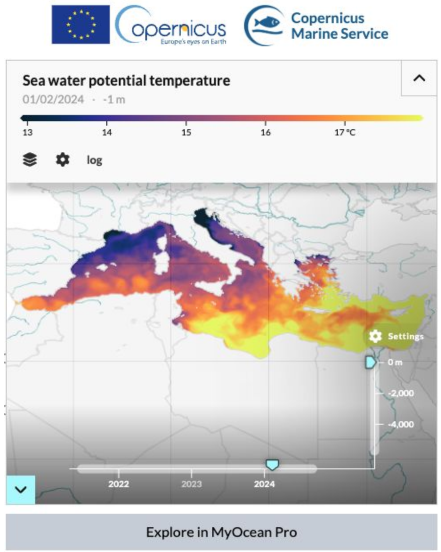
- Daily Med-PHY reanalysis data from January 1987 to December 2021.
- Plus analysis data from January 2022 to April 2024.

Validation Set

- Analysis data from May to June 2024 (check for convergence and overfitting).

Test Set

- Analysis data from July to August 2024.



https://marine.copernicus.eu/

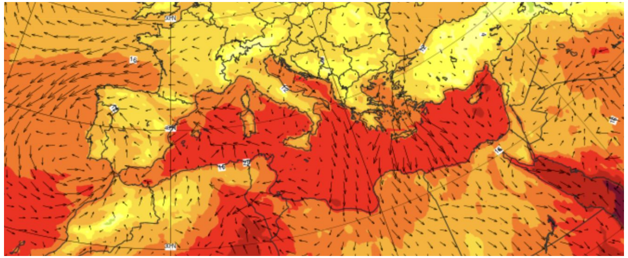
Atmospheric and Boundary Forcing

Atmospheric Forcing

- 4 key drivers: 10-meter zonal and meridional winds, 2-meter temperature, and mean sea level pressure.
- Sourced from ERA5 reanalysis data, bi-linearly interpolated to match ocean grid resolution of 1/24°.
- Includes seasonal forcing features sine/cosine of the day of year.

Boundary Forcing

- Applied at the grid boundary (west of 5.2°W, covering the Strait of Gibraltar).
- Utilizes Mediterranean forecast data for boundary conditions, could perhaps also incorporate global forecasts directly.
- Normally forecast is forced with ECMWF HRES and 10 days long.
- Here: Extended to 15-day forecasts using ENS/AIFS forecasts, with the boundary condition repeated for the last 5 days.



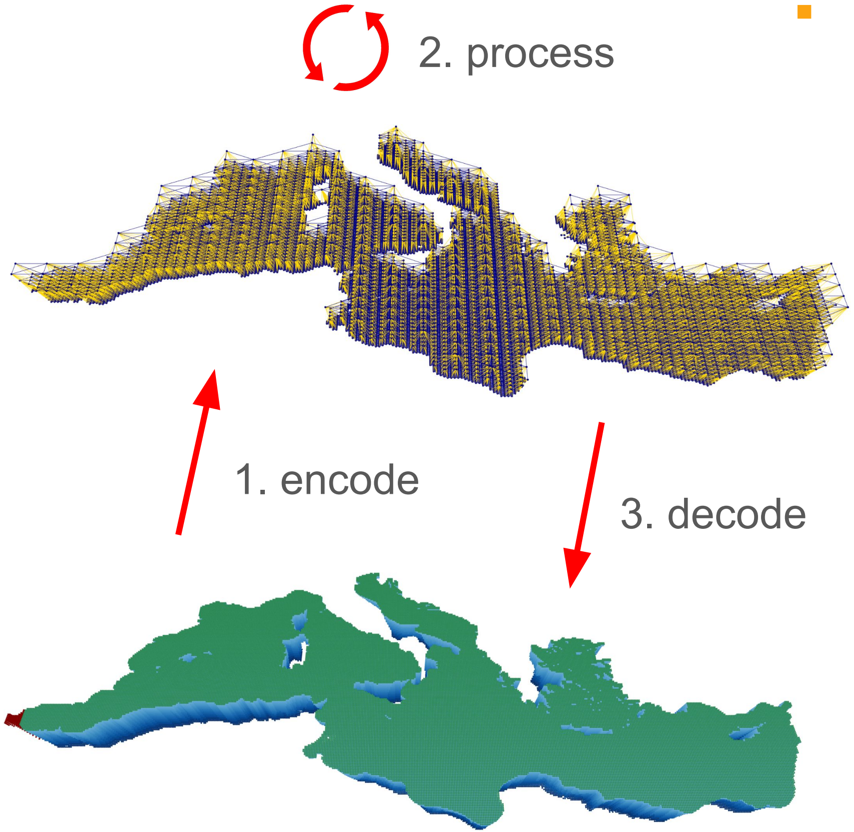
Surface temperature and wind.
https://www.ecmwf.int/

Summary of Propagated Features and Forcing

	Abbreviation	Unit	Vertical Level
Variables			
Eastward sea water velocity	uo	m/s	18 depths
Northward sea water velocity	vo	m/s	18 depths
Ocean mixed layer thickness	mlotst	m	Sea surface
Sea water salinity	so	‰	18 depths
Sea surface height above geoid	zos	m	Sea surface
Sea water potential temperature	thetao	°C	18 depths
Sea water potential temperature at the sea floor	bottomT	°C	Sea floor
Static fields			
Sea floor depth below geoid	deptho	m	Sea floor
Mean dynamic topography	mdt	m	Sea surface
Latitude	lat	°	-
Longitude	lon	°	-
Forcing			
10m u-component of wind	u10	m/s	10 m above surface
10m v-component of wind	v10	m/s	10 m above surface
2m temperature	t2m	°C	2 m above surface
Mean sea level pressure	msl	Pa	Sea surface
Sine of time of year	sin_toy	-	-
Cosine of time of year	cos_toy	-	-

Model Overview

- Several GNNs for meshes have emerged in recent years, e.g.
  - *MeshGraphNet* (2021)
  - *Multi-Scale MeshGraphNet* (2022)
  - Here we use *Hierarchical MeshGraphNet* (2023)
- Quadrilateral mesh used by the model
  - Coarser than the data → efficient processing.
  - Nodes are connected with bidirectional edges to its neighbors horizontally, vertically and diagonally (repeated at 3 different resolutions tripling the distance between nodes).
- GNNs are used to
  1. **Encode** inputs from the data grid to latent vector representations in each mesh node.
  2. **Process** latent node and edge representations using InteractionNet (2016) yielding new latent representations.
  3. **Decode** onto the original sea grid to predict a new state.



Training Objective

- Minimize autoregressive loss over multiple timesteps

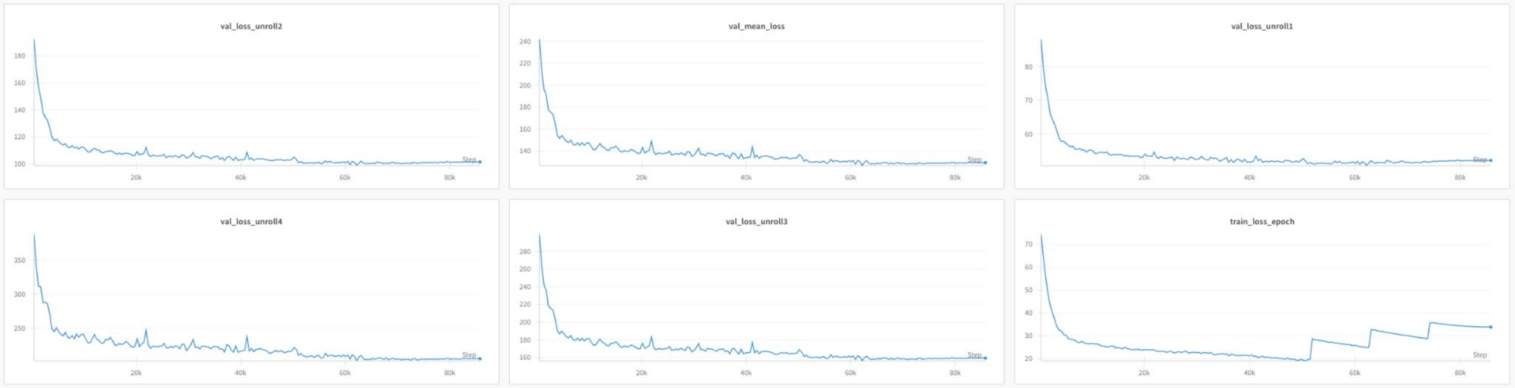
$$\mathcal{L} = \frac{1}{T_{\text{rollout}}} \sum_{t=1}^{T_{\text{rollout}}} \sum_{i=1}^{C} \sum_{l=1}^{L_i} \frac{1}{|\mathbb{G}_l|} \sum_{v \in \mathbb{G}_l} a_v \lambda_i \left(\hat{X}_{v,i}^{t} - X_{v,i}^{t} \right)^2$$

where:

- T_{rollout} is the number of steps in the rollout.
- C is the number of feature channels in the tensor.
- L_i is the number of depth levels for feature i.
- $\mathbb{G}_l$ is the set of ocean grid nodes at depth level l.
- a_v is the latitude-longitude area of grid cell v normalized to unit mean.
- λ_i is the inverse variance of time differences for variable i.

Model Training

- Trained a 5.6M parameter SeaCast model for 200 epochs using a batch size of 1.
- The number of rollout steps is progressively increased to 4 starting at 60% of the total epochs.
- For 200 epochs this translates to updating the steps at epochs 120, 146, and 172 to 2, 3 and 4 rollout steps, respectively.
- Training took 2 days on 32 AMD MI250x GPUs.



Computational Complexity

Med-PHY

- Requires approximately **80 minutes** to run a bulletin, which includes a 1-day simulation and a 10-day forecast, **using 89 CPU cores**.
- Outputs data for **141 vertical levels**.
- Forecast available at both **1-hour and daily mean**.

SeaCast

- **Training took 2 days on 32 AMD MI250x GPUs**. Performed once, possibility to finetune cheaply.
- Produces a complete **15-day forecast in 11.2 seconds** on a single GPU.
- Equivalent to **0.75 seconds per timestep**.
- Forecast **includes 18 depth levels** and provides predictions at a **daily temporal resolution** (dependent on reanalysis).
- Both systems produce outputs at the same **1/24° spatial resolution**.

$$\rho = \rho\,(T, S, p) \qquad \nabla \cdot U = 0 \qquad \frac{\partial p}{\partial z} = -\rho\ g$$

$$\frac{\partial U_h}{\partial t} = -\left[(\nabla \times U) \times U + \frac{1}{2}\nabla\left(U^2\right)\right]_h - f\ k \times U_h - \frac{1}{\rho_o}\nabla_h p + D^U + F^U$$

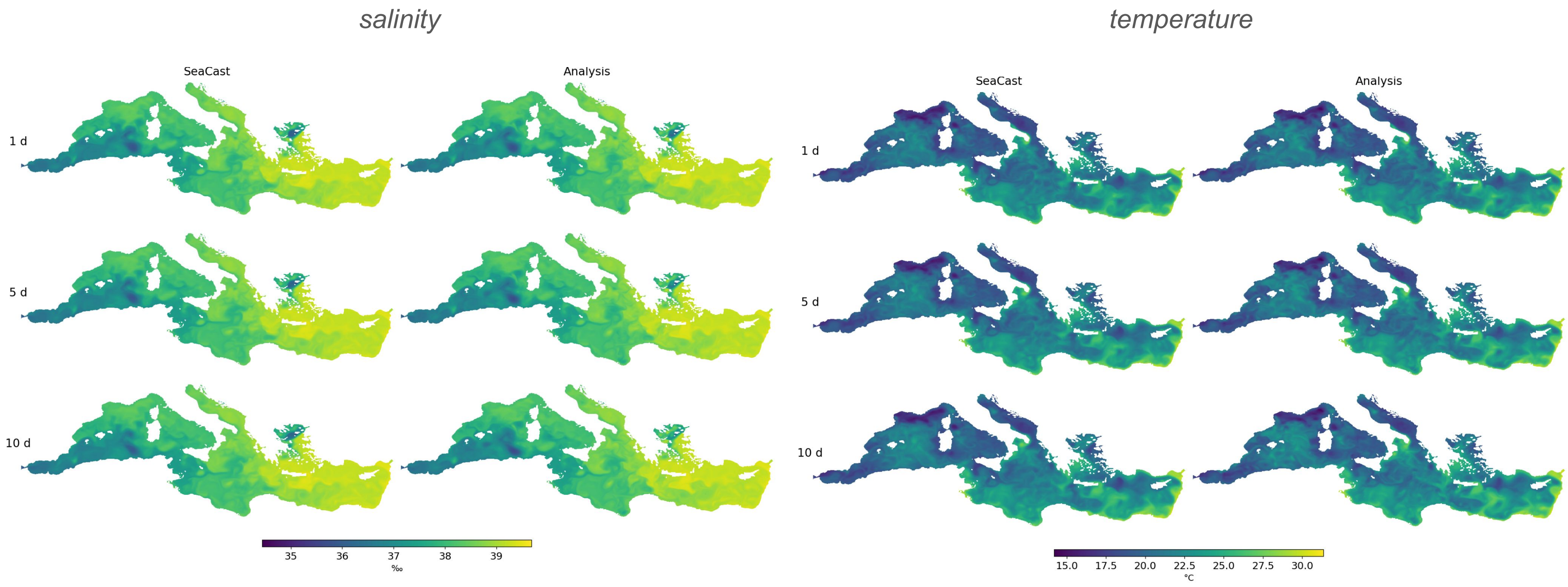
$$\frac{\partial T}{\partial t} = -\nabla \cdot (T\ U) + D^T + F^T \qquad \frac{\partial S}{\partial t} = -\nabla \cdot (S\ U) + D^S + F^S$$

numerical
vs
data driven

input representation of each node

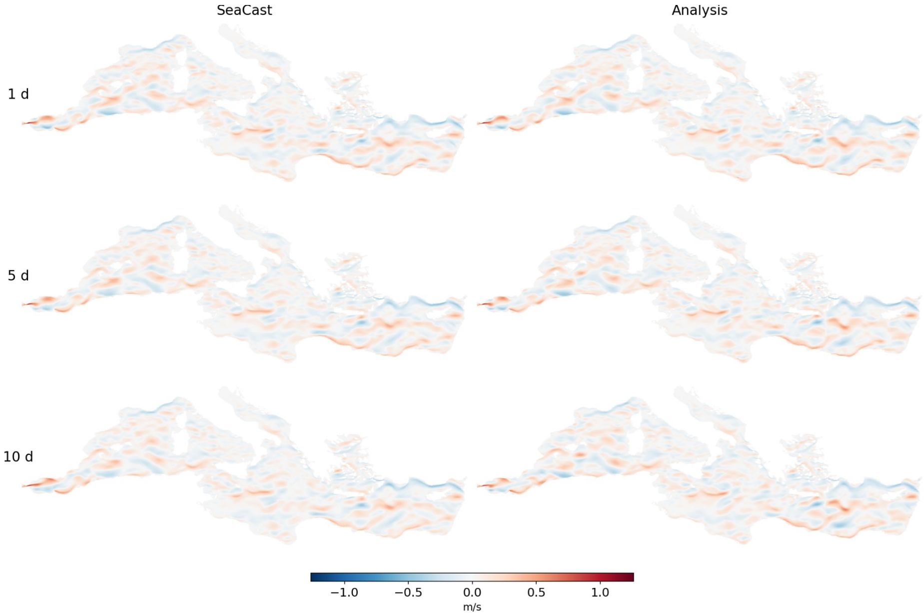
output representation of each node

Salinity and Temperature Forecast at 30 m

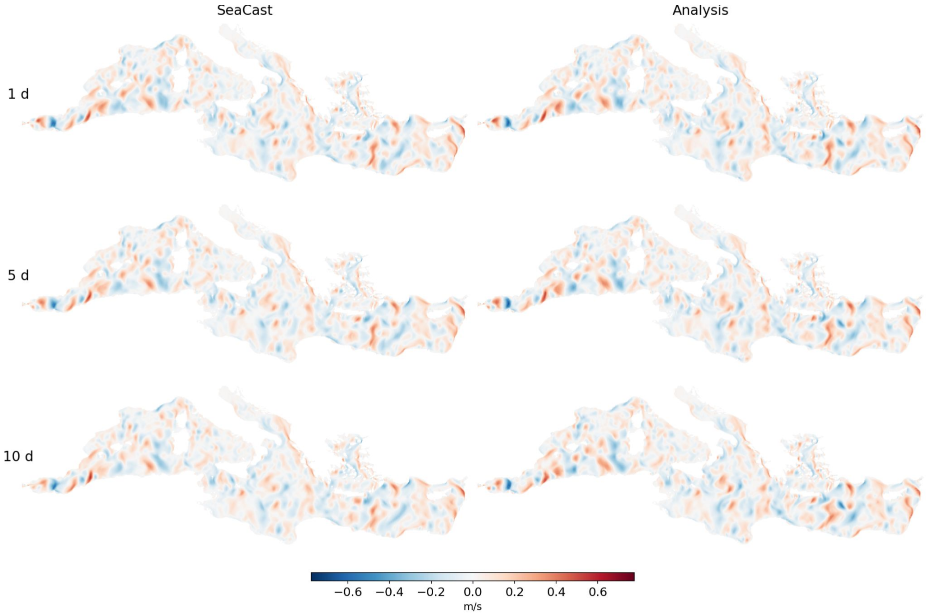


Zonal and Meridional Velocity Forecast at 30 m

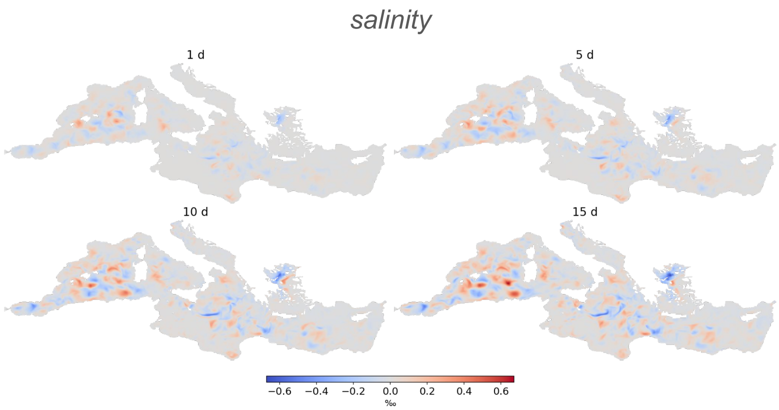
zonal velocity

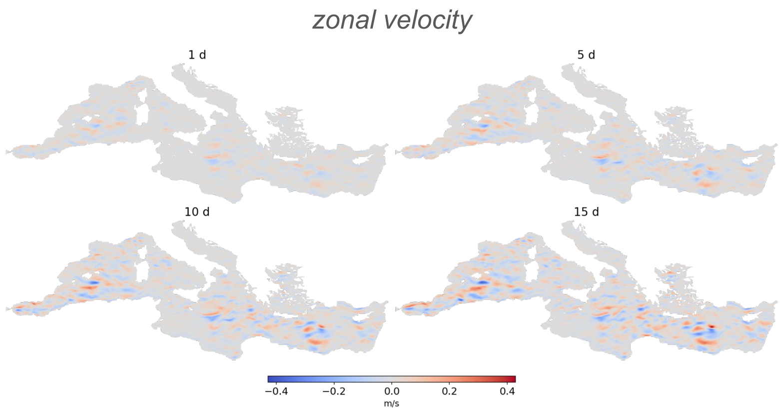


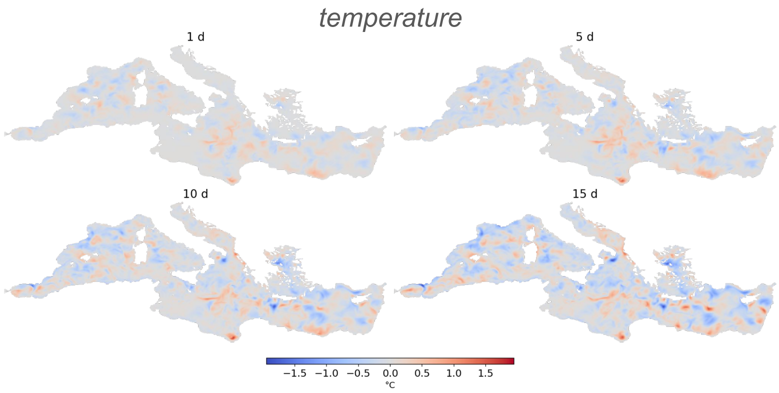
meridional velocity

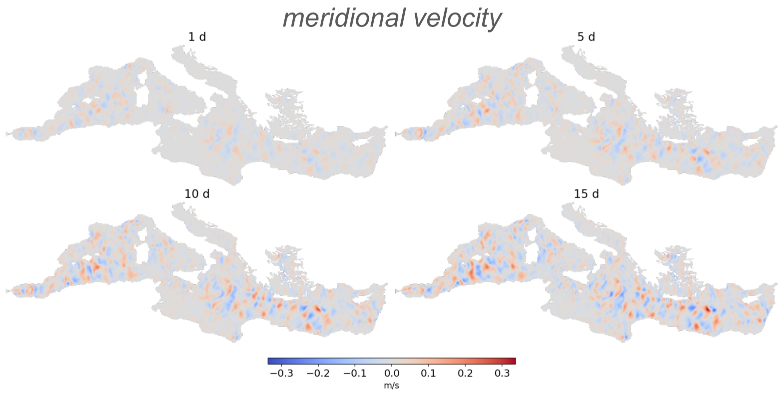


Bias SeaCast-AIFS vs Analysis

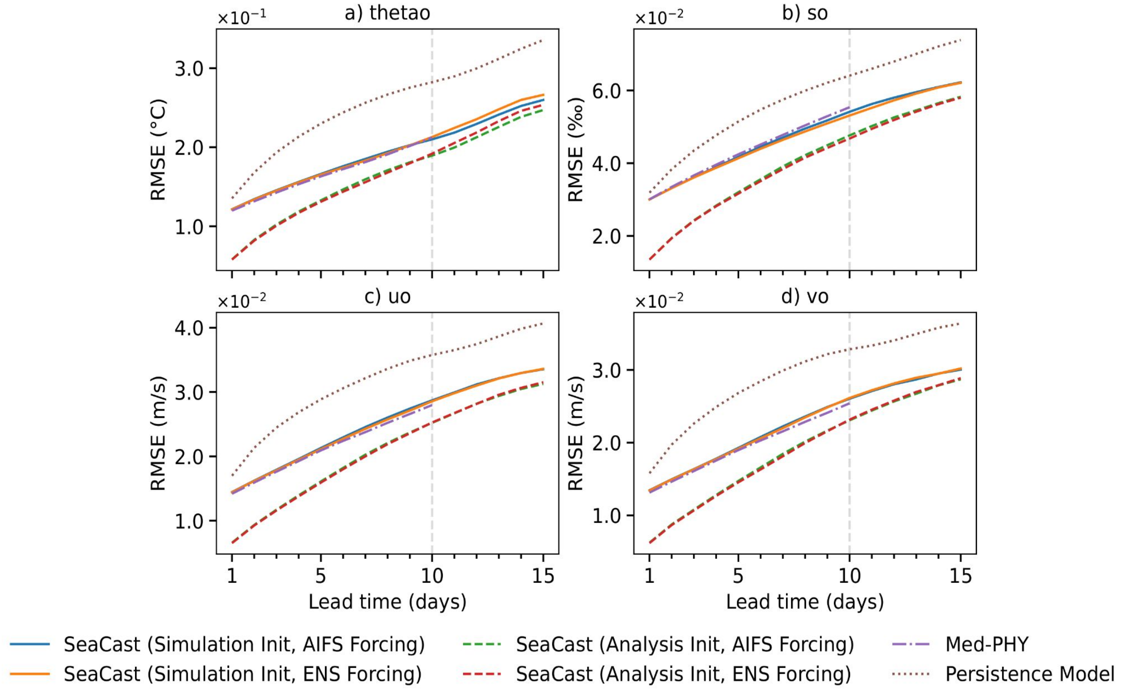




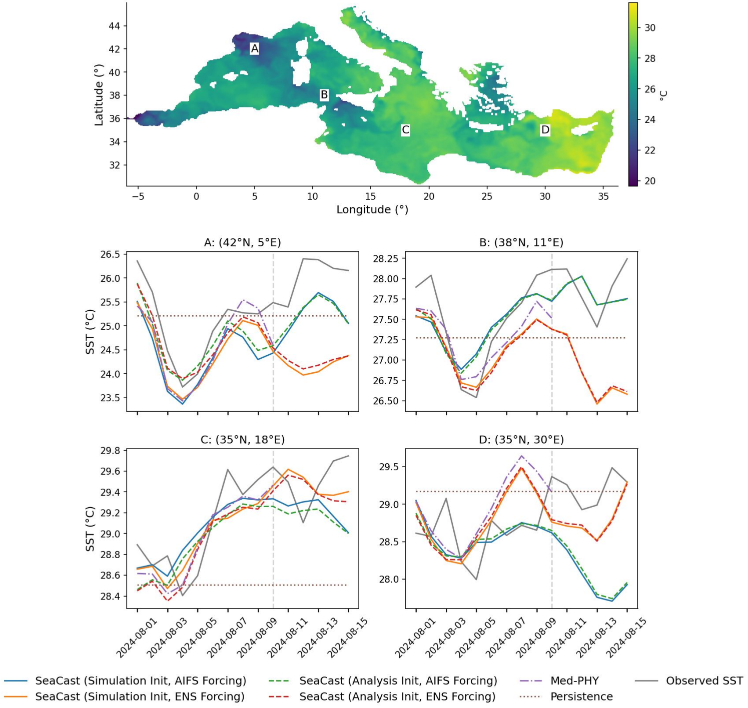




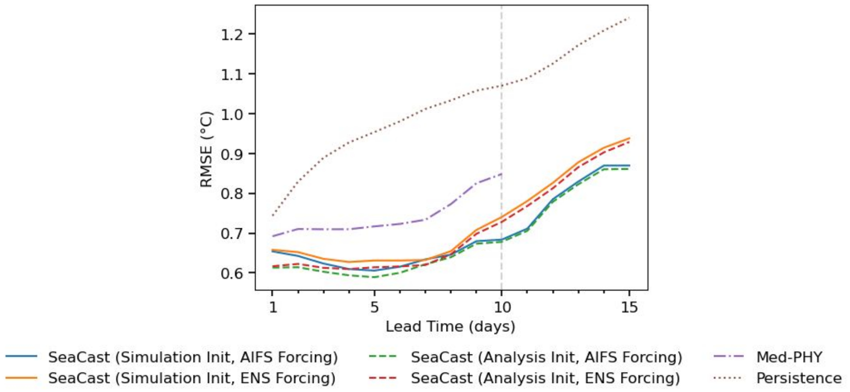
Error vs Analysis for Different Lead Times



Comparison with L4 Satellite SST



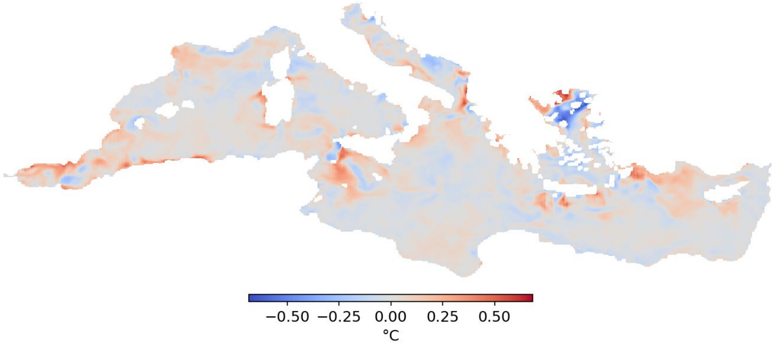
SST verification forecasts issued August 1st, 2024.



SST error at different lead times.

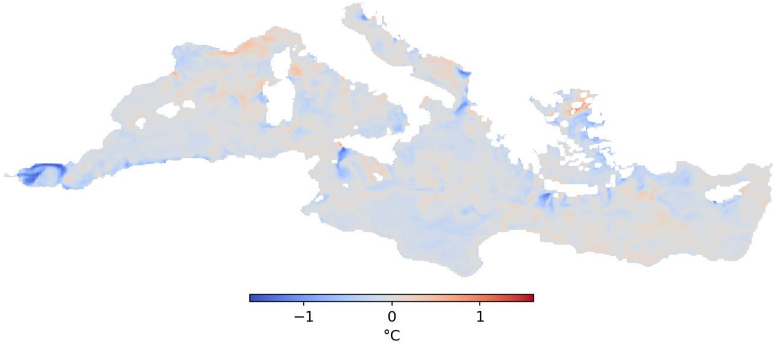
Comparison with L4 Satellite SST

RMSE difference SeaCast-ENS - SeaCast-AIFS



Blue means SeaCas-ENS is better.

RMSE difference SeaCast-AIFS - Med-PHY



Blue means SeaCas-AIFS is better.

Future Work

- Personally:
    - Force Dardanelles (open boundary in forecast)
    - Look into training a larger model using e.g. mixed precision training
    - Longer evaluation (currently a month)
- Data-driven sea forecasting more broadly:
    - Higher temporal res for the reanalysis → higher res data driven forecast.
    - Tidal input used in analysis/forecast → also in reanalysis.
    - Include more depth levels.
    - ML forecast of waves and biogeochemistry also possible given enough data.
    - Possible to do probabilistic / ensemble forecast.
    - Ocean modeling could benefit from foundation models.
        - E.U. WeatherGenerator https://www.ecmwf.int/en/about/media-centre/news/2024/weathergenerator-project-aims-recast-machine-learning-earth-system

Thank you.

preprint

https://arxiv.org/abs/2410.11807

code

https://github.com/deinal/seacast