Oceanographic predictions: How HPC can help train reliable AI models

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AI FOR WEATHER & CLIMATE

How Machine Learning Boots Forecasting

Webinar 13/11/2024 10:00 CET

Problem

- **Oceanographic Forecasting Importance:** Vital for improving maritime transportation efficiency and reducing emissions.
- **Challenges:** Traditional numerical models have reached their accuracy limits due to the chaotic and complex nature of ocean physics and high computational demands.
- **Goal:** Introduce AI models to improve Significant Wave Height (SWH) prediction*.

AI Opportunities: Improve forecast precision, reduce environmental impact, and support safer maritime operations.

*Significant Wave Height is the average height of the highest one-third of waves in a given wave spectrum, commonly used in oceanography to describe wave conditions and forecast marine environments.

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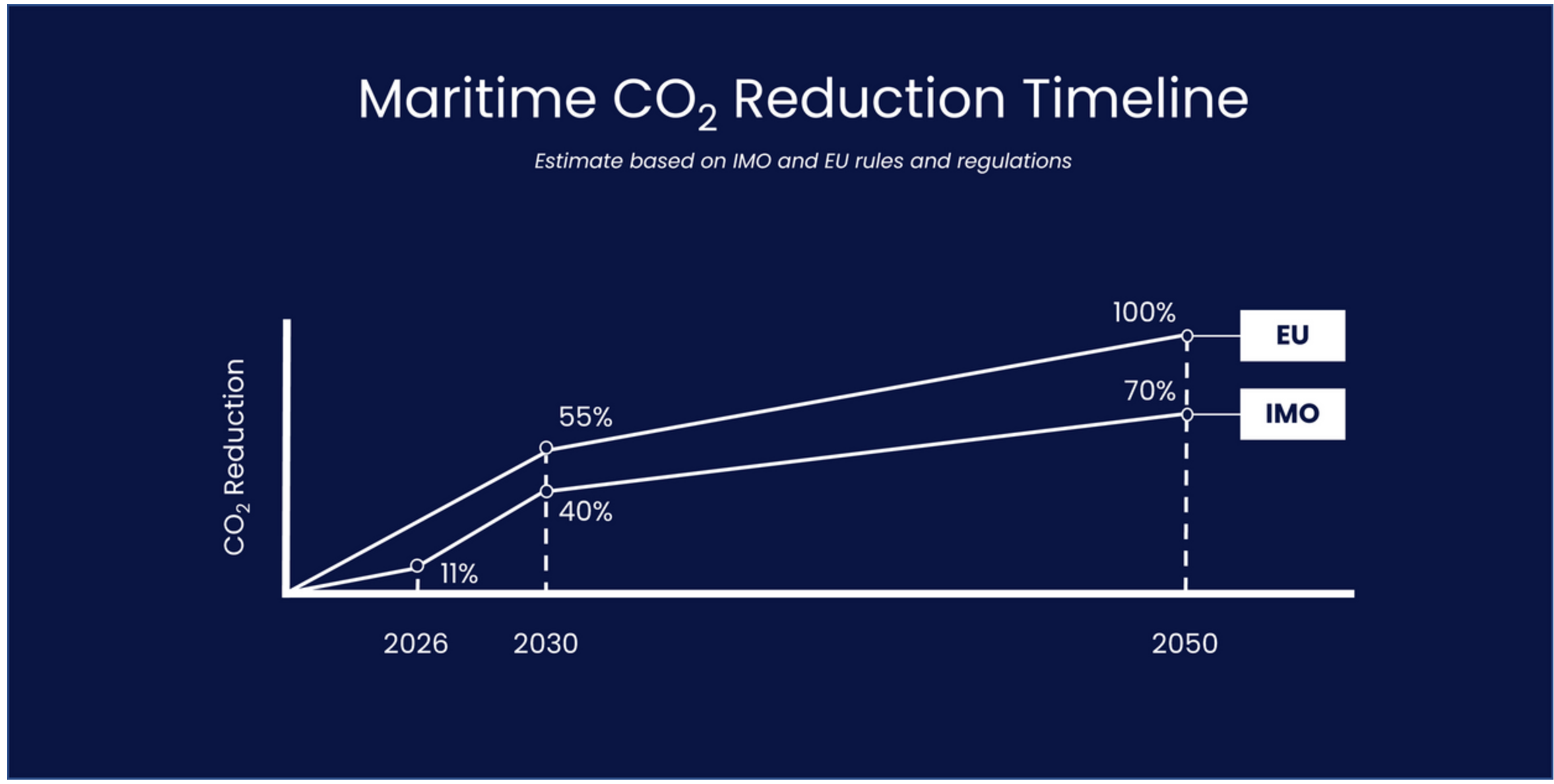
Problem

Shipping contributes ~3% of global GHG emissions

Regulations are driving reduction

near-zero GHG by 2030

net-zero GHG by 2050



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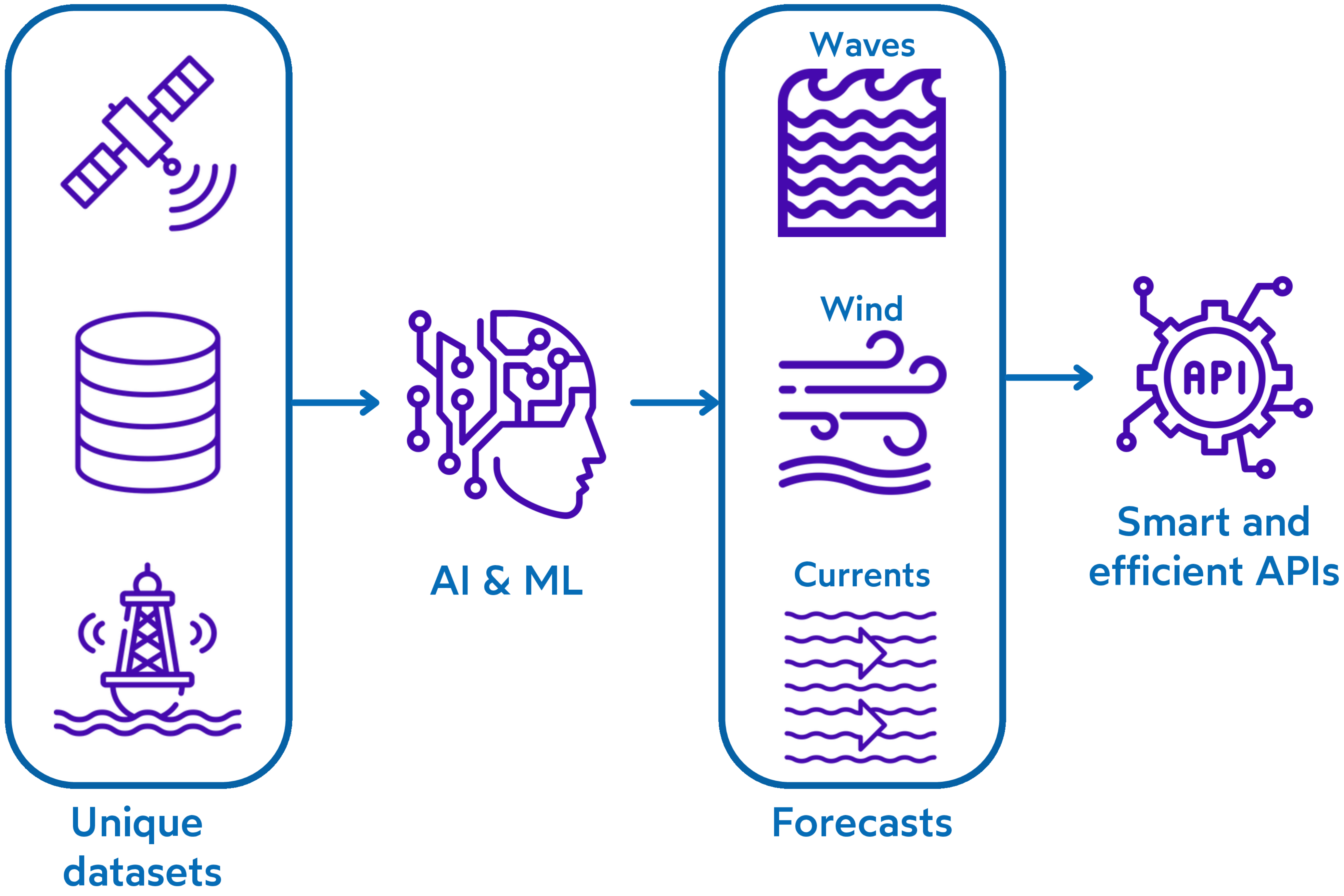
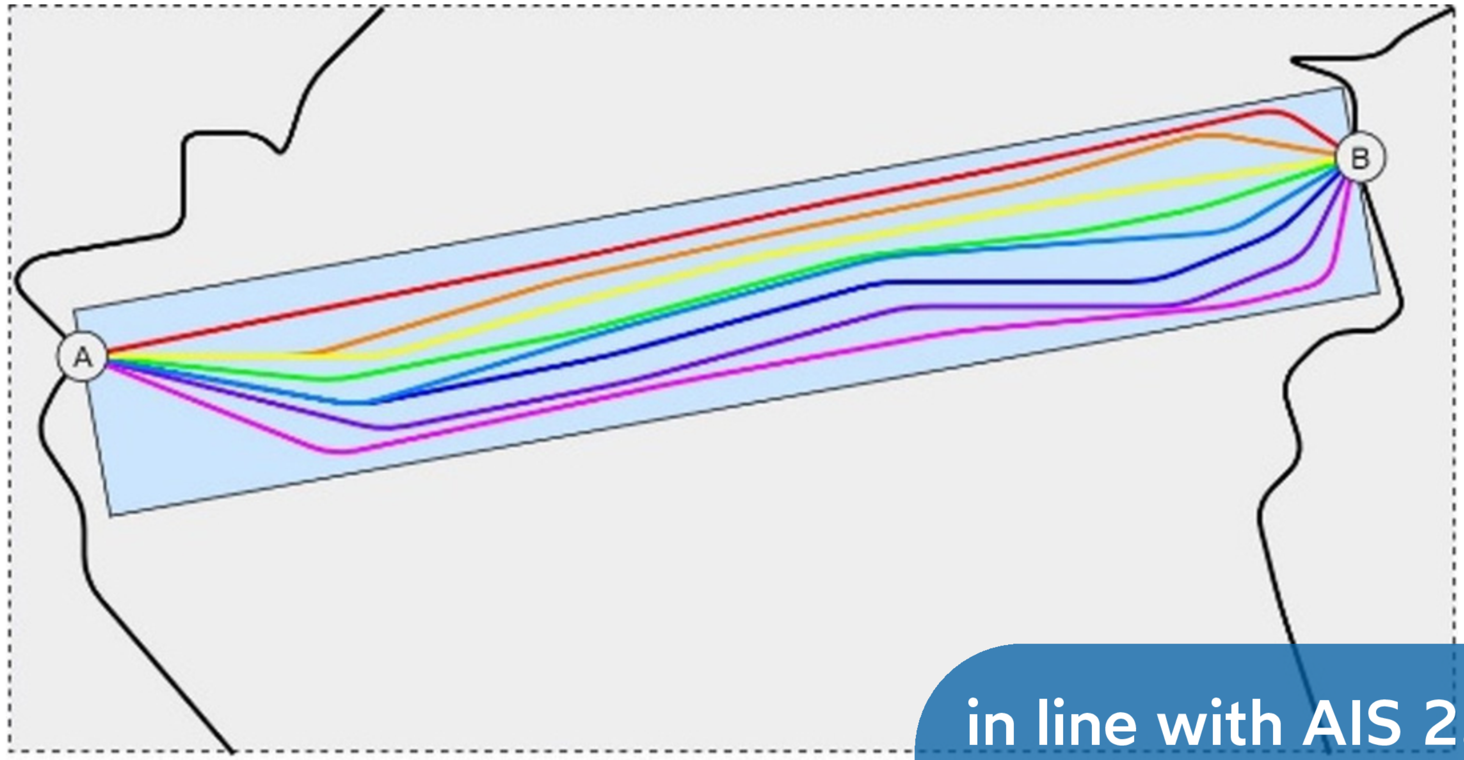
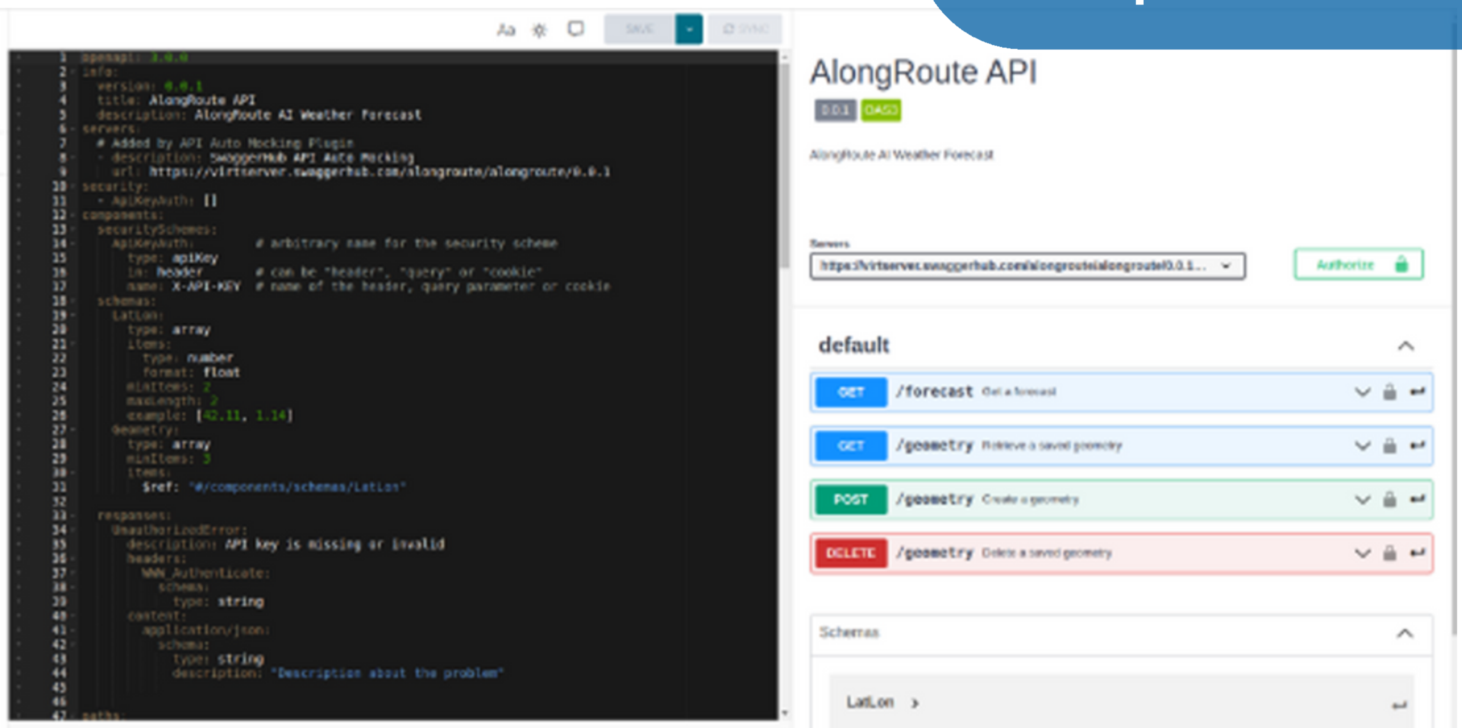
Solution

We produce and deliver data with great efficiency





in line with AIS 2.0 requirements



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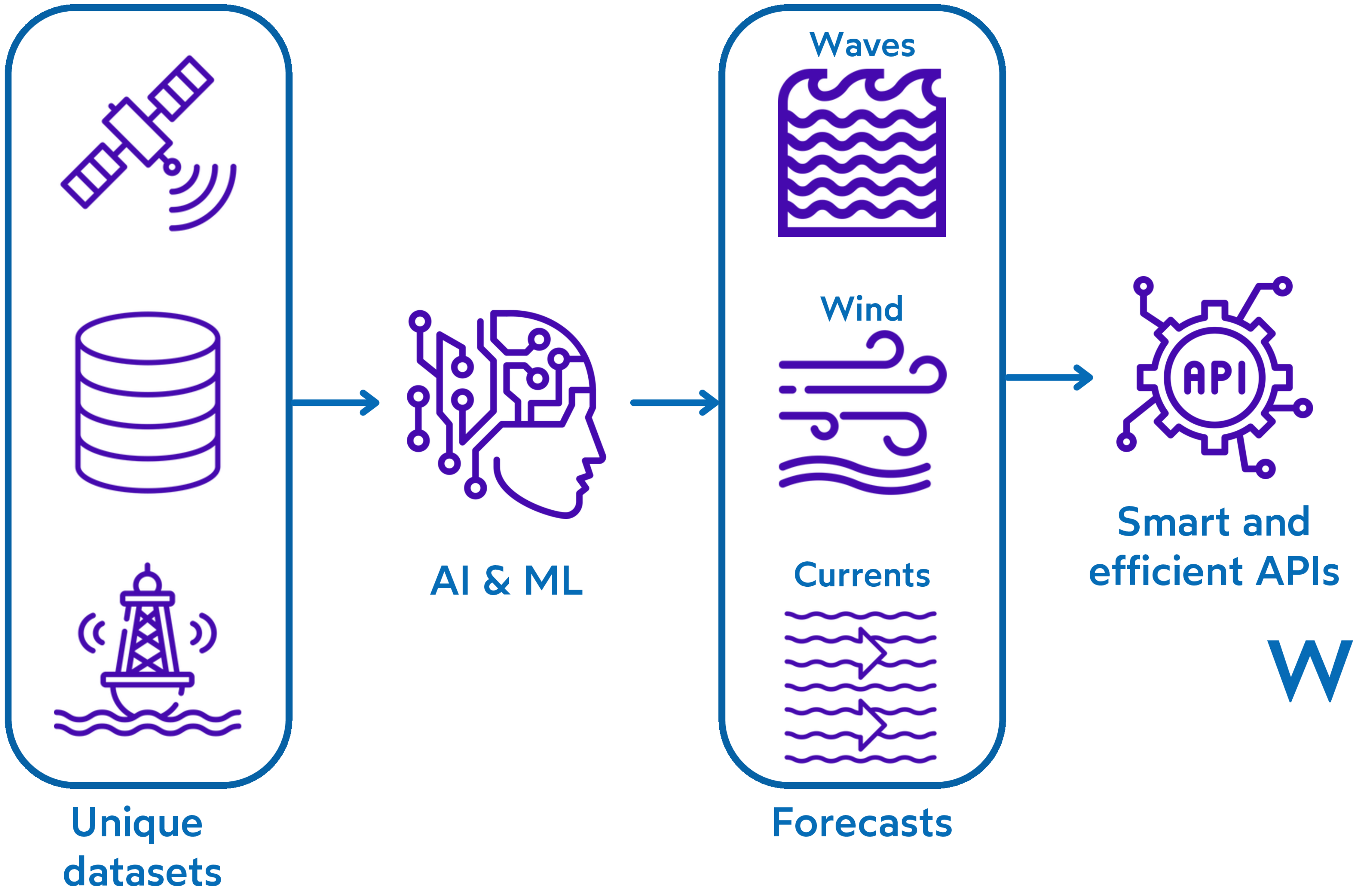
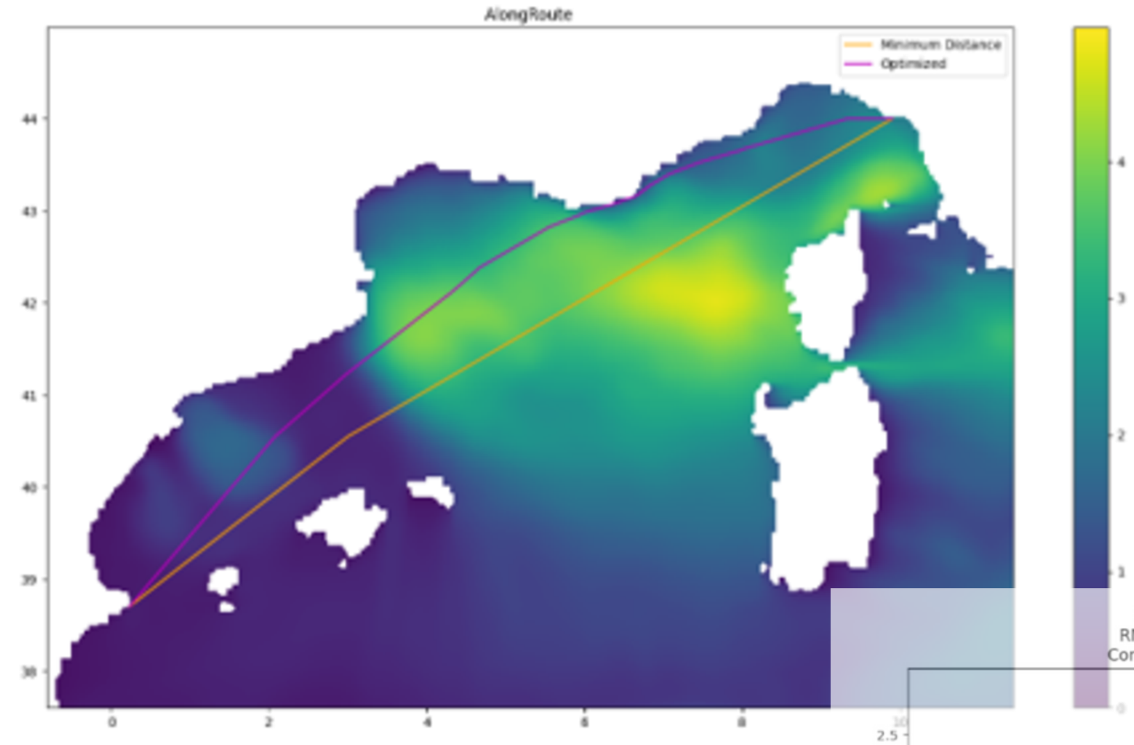
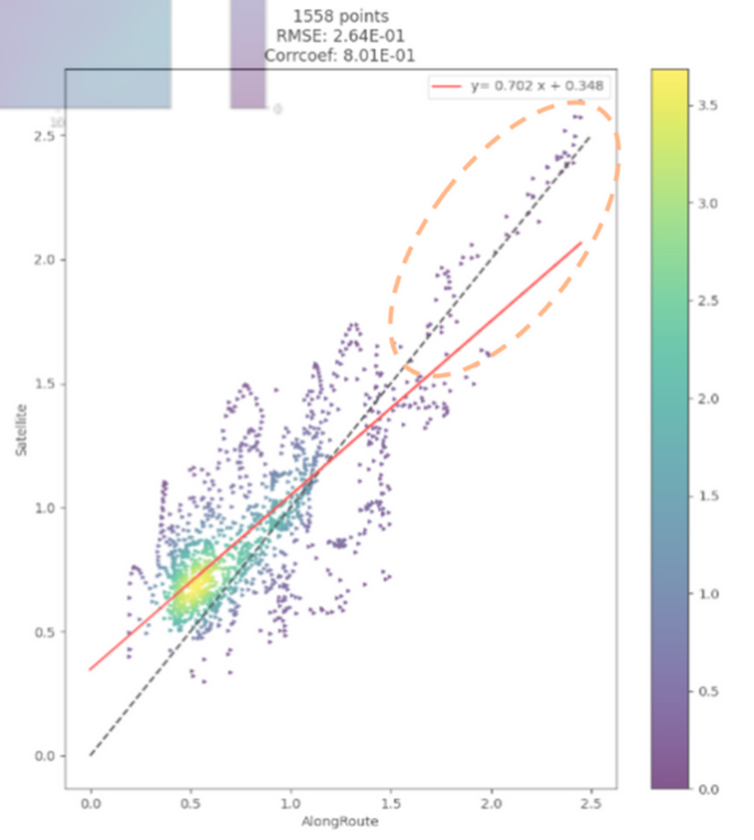
Solution

We protect our advantage with trademarks, copyright and trade secrets







We can go up to

10%

in better forecasts

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Continuous R&D – serving business needs

CNNs Convolutional Neural Network

→ Suitable for 1-hr ahead forecasts, outperforming CMEMS in high waves

→ Forecast horizon **not** suitable for shipping companies

→ R&D including spatiotemporal dependencies

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Continuous R&D – serving business needs

1. Extensive training on larger amount of input data and crucial variables, and
2. Spatiotemporal charateristics that allow to extend the forecast horizon

Proceedings of the First EuroHPC user day

HPC-Driven oceanographic predictions with Graph Neural Networks (GNNs) and Gated Recurrent Units (GRUs)

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[b]AlongRoute, 15 km N.R. Thessaloniki-Moudania, 57001 Thermi, Greece

Continuous R&D – serving business needs

Spatio-temporal characteristics that allow to extend the forecast horizon.

Spatial → Graph Neural Networks

Pangu Weather by Huawei
GraphCast by Deepmind
MetNet (and MetNet-2) by Google

Spatial → Graph Neural Networks

Temporal → Gated Recurrent Units

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Continuous R&D – serving business needs

- **HPC Utilization:** Vienna Scientific Cluster (VSC5) for model development and training.
- **Data Sources:** CMEMS and CDS oceanographic and atmospheric datasets.
- **Model:** GNN-GRU hybrid combining spatial and temporal data analysis.

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Model Architecture

- Hybrid Model: GNNs for spatial relationships, GRUs for temporal dependencies.
- Framework: PyTorch with Optuna for hyperparameter optimization.
- Training Setup: NVIDIA A100 GPUs, 559 million data points processed in 13 hours.
- Frameworks: PyTorch, Optuna for hyperparameter tuning

Reanalysis data, their characteristics and the number of selected variables to train the model

Reanalysis Data	Spatial Resolution	Temporal Resolution	Number of total variables	Number of Selected Variables
MEDSEA_MULTIYEAR_WAV_006_012 (CMEMS)	0.042° x 0.042°	Hourly	18	5
MEDSEA_MULTIYEAR_PHY_006_004 (CMEMS)	0.042° x 0.042°	Hourly	10	2
UERRA (CDS)	5.5 km x 5.5 km	6-hourly	19	3

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Training Data Split: 60% training, 20% validation, 20% testing.

Performance Metrics against test data:

- **MAE: 0.0071**
- **R-squared: 0.98**
- **RMSE: 0.015**

Forecasting: Three models for predicting 6, 12, 18, 24 hrs ahead.

Training Area

Model Architecture

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- Framework: PyTorch with Optuna for hyperparameter optimization.
- Training Setup: NVIDIA A100 GPUs, 559 million data points processed in 13 hours.
- Frameworks: PyTorch, Optuna for hyperparameter tuning

Challenges: Memory handling during pre-processing, temporal and spatial aggregation.

Solution: Utilized GPUs with 512 GB RAM, cleaned data frames efficiently.

Validation Results

Validation Strategy:

Test Period: Used out-of-training data with challenging sea conditions

Comparison: Reanalysis data from CMEMS and satellite SWH

Findings: Captured general wave patterns well, but with overestimation in coastal areas.

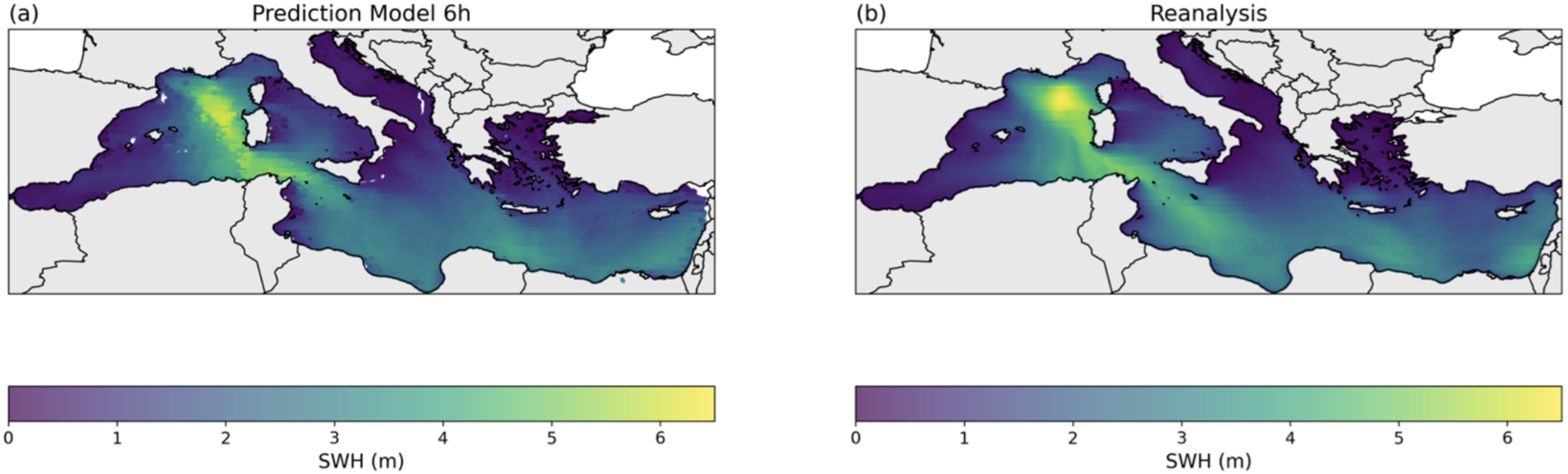

Figure. (a) Model prediction on 14/1/2014; (b) Reanalysis data of SWH for the same time

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Validation Results

- **A distinct clustering of overestimated values was evident, particularly in regions with complex coastlines.**
- **To address these challenges, buffer zones were implemented around the islands to mitigate the buildup effect and improve prediction accuracy in coastal areas.**

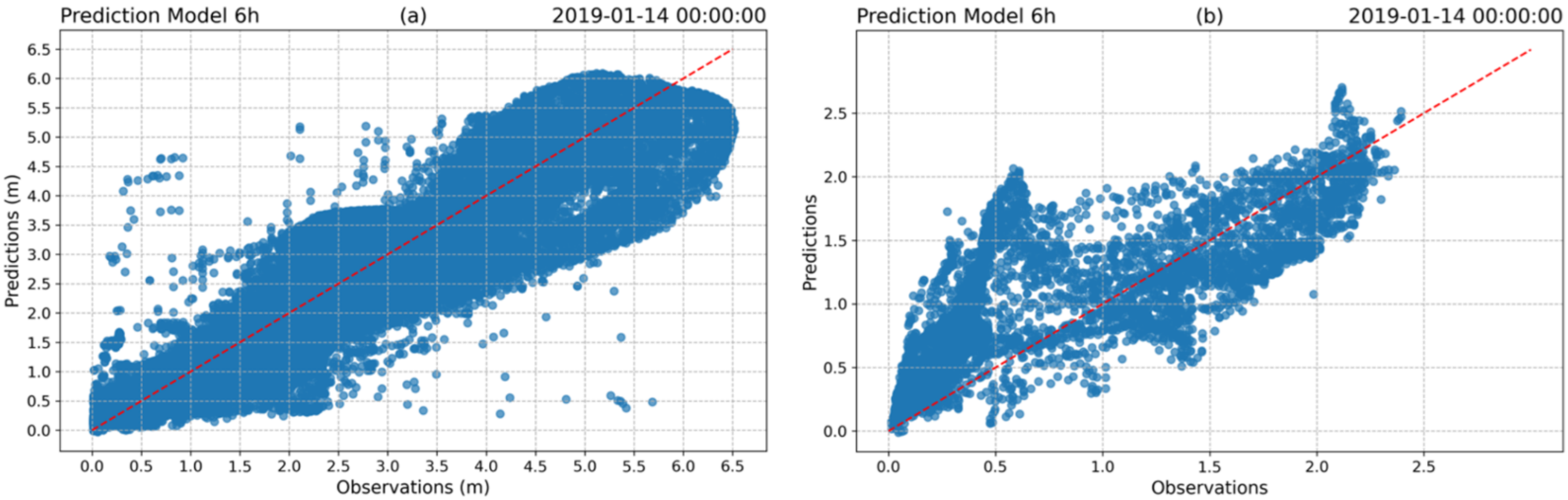

Figure. (a) Scatter plot of predicted versus reanalysis data for Mediterranean (with buffer zone round coastlines); (b) Scatter plot of predicted versus reanalysis data for Aegean (without buffer zone around coastlines).

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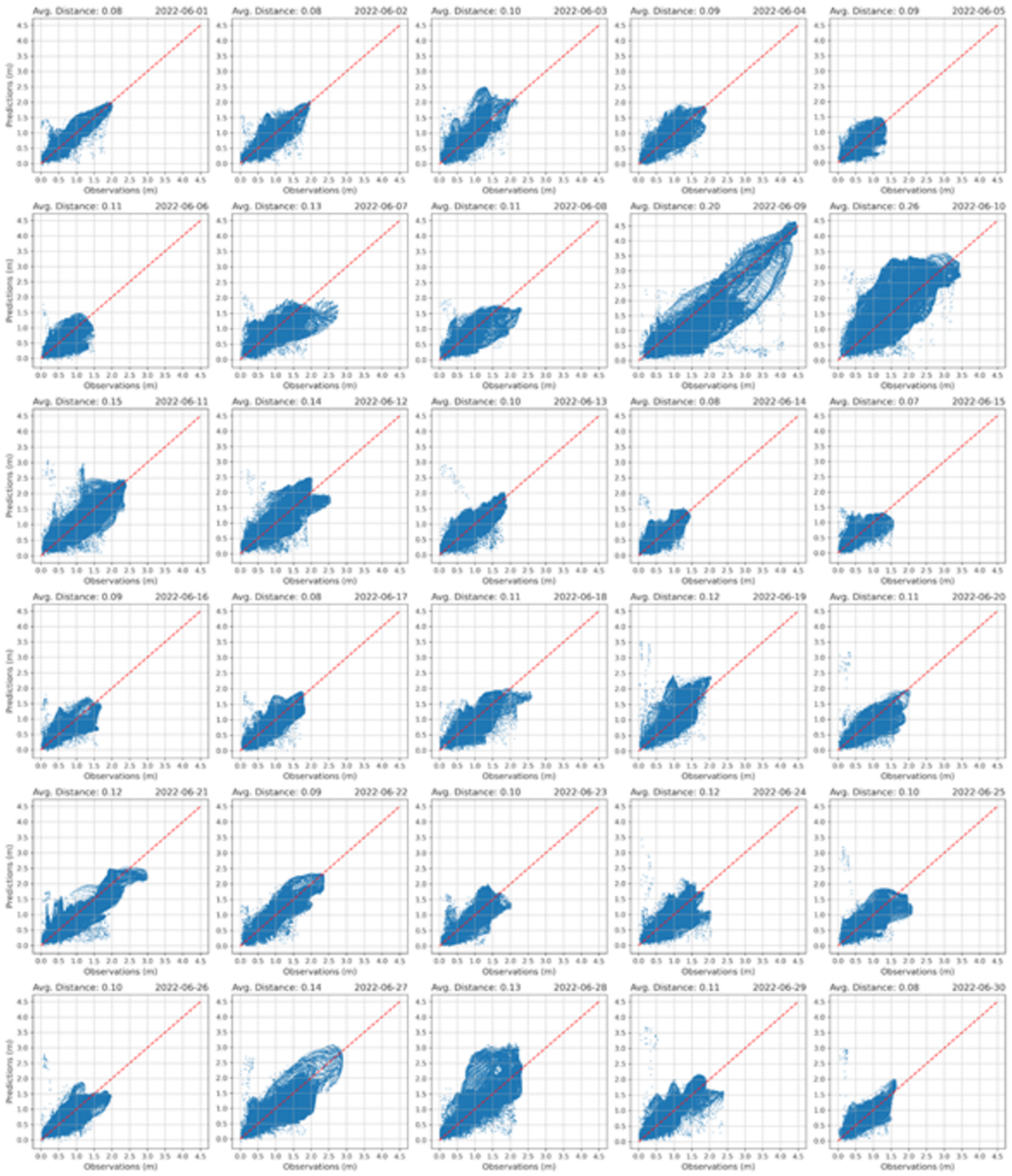
Validation Results

One month of 6-hourly forecasts with GNN-GRU against renalysis (June 2022)



RMSE (avg. value = 0.22)
MAE (avg. value = 0.16)
MBE (avg. value = 0.01)

One month of 6-hourly forecasts with GNN-GRU against Global Ocean L3 Spectral Parameters From Nrt Satellite Measurements (June 2022)

RMSE (avg. value = 0.38)
MAE (avg. value = 0.32)
MBE (avg. value = 0.13)

Conclusion and future work

Summary: The GNN-GRU hybrid model demonstrates significant potential in enhancing the accuracy and reliability of Significant Wave Height (SWH) forecasting, achieving high precision in complex oceanographic conditions.

Impact: AI and HPC together can significantly advance maritime operations and environmental sustainability.

Future Work: The team is actively developing a Data Assimilation Strategy to achieve more precise forecasts.

Operational Testing with the Shipping Industry: Real validation of our operational setup directly with industry partners, gathering real-world feedback to refine our solution and better address industry needs.

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Thank you

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