





# Challenges and future directions in ocean analysis and forecasting

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- 1. User needs and scientific challenges
- 2. Ongoing developments and future directions:
  - Observing systems impact and design
  - Ocean and coupled modelling
  - Ocean and coupled data assimilation
  - The role of machine learning & digital twins
- 3. Summary and conclusions









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## **1. User needs and scientific challenges**

#### **1.1 User needs - overview**

- High spatial and temporal resolution needed to resolve the main features of interest.
- High *accuracy*.
- Uncertainty quantification and probabilistic forecasts.
- Many user cases require consistent *coupled forecasts* of ocean (O), waves (W), atmosphere (A) (and biogeochemistry (BGC)).
- Many users need *timely* data with frequent updates.
- Requirement for *consistent forecast and reanalysis*, e.g. design and operations, seasonal forecast calibration.

Use Category	Example Cases	Components	Forecasts / Past time-series
Coastal Flood	Coastal Flood Coastal Boundary Conditions	O, W, A	Both
Marine Safety and NetZero	Offshore Operations Safe/Efficient Navigation Beach safety	O, W, A	Both
Marine Sourced Energy	Offshore Renewable Energy Generation Ambient Water Characteristics	O, W, BGC, A	Both
Marine Accident Response	Search and Rescue Marine Pollution Response Coastal Boundary Conditions	O, W, BGC, A	Both (short- term past)
Marine Environment Monitoring	Marine Ecosystem Health Monitoring Climate Change Physical Impacts Monitoring SST/Sea-Ice Reference Dataset	O, W, BGC, A	Past
(Coupled) Weather, Marine and Climate Predictions	Weather and Seasonal Forecasts Marine heatwave forecasts Coastal Boundary Conditions	O, W, A	Both

#### Use case examples







#### **1.1 User needs – high resolution**

- Increasing resolution to resolve key features
- Example from coupled ocean/wave forecasting system at 1.5 km resolution
- Impact on internal tides, topographic steering, coastline effects and resolving eddies



2022 Jun 08, 12:00

Eddies and internal waves in SW approaches, impact on wave field

AMM15

From ~7km -> 1.5 km resolution Increased structure and intensity in surface current fields

Surface currents

MAMM7







unesco

## 1.1 User needs – uncertainty quantification and probabilistic forecasting

Ensemble GIOPS

Mean Probability Occurence (glb.avg. = 0.08592194193241315)





Any downstream application and costbenefit analyses benefits from probabilistic predictions

Example: Probability of occurrence of sound ducts from ensemble ocean predictions with stochastic physics

Courtesy of Drew Peterson (ECCC)







#### **1.1 User needs – consistent earth system predictions**

Regional atmosphere/ocean coupled impacts:

Atmosphere

Coastal She

Sea (NEMO)

- Atmospheric conditions (persistent anticyclonic conditions) generated a marine heatwave (MHW) in the Northwest European Shelf Seas in June 2023.
- Coupled regional environmental prediction system including ocean, waves, atmosphere, land components used to understand the development of the MHW.
- UK broke its record June monthly temperature by +0.9 °C, of which 0.6 °C came from the feedback of the MHW on the atmosphere temperature over land.
- Regional NWP quality improved using time-varying SSTs from regional ocean forecasting system even for short 36 h forecasts, during the MHW.



#### Impact of MHW on 1.5 m air temperature



#### Ocean Predict

River flow

Waves

Berthou et al., 2024





MHW/SST anomalies in June 2023

Does the increase in spatial resolution always benefit the forecasting systems? The conundrum of the unconstrained scales (for assimilation but also validation)



Description	SLA MAD (cm)	SST MAD (K)	
2.5 km nature run	13.1	1.31	
10 km nature run	12.7	1.23	
2.5 km reanalysis	7.8	0.41	
10 km reanalysis	6.6	0.38	
2.5 km upscaled	7.7	0.40	

From Sandery and Sakov 2017: Ocean forecasting of mesoscale features can deteriorate by increasing model resolution towards the submesoscale



From Thoppil et al. 2021: Ensemble forecasting greatly expands the prediction horizon for ocean mesoscale variability







Does the increase in spatial resolution always benefit the forecasting systems? The conundrum of the unconstrained scales (for assimilation but also validation)



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From Souopgui et al. 2020: Multi-scale assimilation of simulated SWOT observations







Does the increase in spatial resolution always benefit the forecasting systems? Many "immortal" biases despite the incremental spatial refinements



From Farneti et al., 2022: Improvements and persistent biases in the southeast tropical Atlantic in CMIP models







Representation of high-frequency processes is challenging in most current analysis and forecast systems

#### **Diurnal Cycle**



#### **Near-Inertial Oscillations**

Left: assimilation of diurnal SST to improve diurnal cycle representation (Storto & Oddo, 2019) and importance in forecasts (Salisbury et al., 2018).

**Right**: wave-induced surface stresses and the Coriolis-Stokes force necessary to represent near-inertial oscillations (Rohrs et al., 2019)









Technical challenges:

#### New HPC architectures (ARM, GPU, mixed, and associated parallelization paradigms)

Efficient programming languages and

the implications for academy and young

researchers, and DTO-related

developments



(from <a href="https://www.youtube.com/watch?v=qQXXI5QFUfw">https://www.youtube.com/watch?v=qQXXI5QFUfw</a>)















## 2. Ongoing developments and future directions

2.1 Observing systems impact and design

2.2 Ocean and coupled modelling

2.3 Ocean and coupled data assimilation

2.4 The role of machine learning & digital twins

## 2.1 Observing systems – impact and design

Various methods to assess the impact of observing systems in ocean forecasting systems:

- Observing System Experiments (OSEs)
  - Existing observations are removed from the assimilation and the impact assessed.
- Observing System Simulation Experiments (OSSEs)
  - Synthetic observations generated from a high-resolution model (nature run) and assimilated into a different model.
  - Used to assess impact of existing and future observing networks and to aid in observing system design.
- Other methods available (not covered here) include (see for example Edwards et al., 2024):
  - Representers
  - Array modes
  - Forecast Sensitivity to Observation Impacts (FSOI).





## 2.1 Observing systems – impact and design

#### Synergistic Observing Network for Ocean Prediction (SynObs)

- SynObs is the Project of the United Nations (UN) Ocean Decade under the UN Decade program ForeSea to seek the way to get maximum synergy from the combination among various observation platforms in ocean predictions.
- SynObs is collaborating with CLIVAR/GSOP, WCRP/S2S, Argo, TPOS, and UN Decade program "Ocean Observing Codesign" led by GOOS, etc.
- SynObs is now promoting a coordinated OSEs using various ocean and coupled atmosphereocean prediction systems.
- Early results are published in the special issue of Frontiers in Marine Science

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Fujii et al., 2024

Difference of SSH muti-system ensemble spread calculated from OSE outputs of UKMO, ECCC, JMA, JAMSTEC, ECMWF.

#### NoArgo NoAlt CNTL CNTL 75N · 75N -45N -45N 15N · 15N 155 -155 455 -455 -755-755 -----120F 120E 60F 0.02 0.05 -0.02 -0.01 0.00 0.01 0.10 -0.10

- Left panel: Assimilating satellite altimetry data reduces the uncertainty of the SSH fields.
- Right panel: The uncertainty of the SSH fields are further reduced when Argo data are assimilated in addition to the altimetry data.







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### **2.1 Observing systems – impact of SWOT using OSEs**

SWOT data available in its 21-day repeat orbit since late July 2023.









## **2.1 Observing systems – impact of SWOT using OSEs**

SLA Error : SLA (Adding SWOT) – SLA (Witout SWOT), Sep 2023-March 2024



<u>Adding SWOT:</u> more mesoscale structures everywhere, positive impact in all regions

Model error relative to the non assimilated Saral/Altika data

	Open Ocean		Coastal region	
	Analysis	Forecast	Analysis	Forecast
Low variability	15.1%	12.9%	13.4%	10.5%
High variability	14.5%	10.6%	14.0%	10.8%



Impact on SLA error variance in MOI system

M. Benkiran, MOi







## 2.1 Observing systems – future altimeter constellation OSSEs

• Assessing the impact of two possible *future constellations* for Sentinal-3 Next Generation:

Zoom of obs coverage in Gulf Stream region

12 nadir altimeters

•

- 2 wide swath altimeters (WiSA)
- OSSEs using the global Met Office system and the MOI system, both at 1/12° resolution.





- Both constellations resulted in large improvements in SSH and surface velocities.
- Met Office system benefitted more from the 12-nadir constellation
- MOI benefitted more from the 2-WiSA constellation.



King et al., 2024 Benkiran et al., 2024







## 2.1 Observing systems – future altimeter constellation OSSEs

- Results on previous slide were from OSSEs where the WiSA observation errors had no correlated component.
- Including correlated observation errors (without representing it effectively in the DA) led to degradations in the surface currents.
- We therefore need quick pre-processing of WiSA data to remove correlated errors, and/or deal with them directly in the DA.
- ESA are now planning that S3-NG will have 2 WiSAs (and nadir altimeters).
- Need to prepare OOFS to make the most of this type of data make good use of SWOT while it's flying to improve its assimilation.





#### Sentinel-3 NG-TOPO concept:

- Constellation of 2 large satellites with ka-band acrosstrack interferometer, a la SWOT.
- Constellation can achieve global 5-day revisit with an effective ocean spatial resolution of 50 km.
- Launch early 2030s.



King et al., 2024







## 2.1 Observing systems – future satellite measurements of surface currents

- The ESA A-TSCV project aimed to demonstrate the potential impact of satellite TSCV data on OOFS and define our requirements.
- Two operational global ocean forecasting systems were developed to assimilate these data and assess impact in a set of coordinated OSSEs: MetO and MOI.



Change in RMSE of surface zonal velocity from assimilating TSCV data (blue => reduction)



- Particles were seeded every 1/4° and advected by the model surface velocities using OceanParcels.
- The impact of the TSCV assimilation on the error in particle locations after different advection times is shown.





Waters et al., 2024a and 2024b Mirouze et al., 2024









## 2.1 Observing systems – future satellite measurements of surface currents

#### Future directions

- Support the ODYSEA mission proposal (cf. Remy et al.) and other missions for measuring surface currents.
- Develop improved assimilation methods for this type of data, e.g.
  - Developing different control variables (streamfunction and velocity potential) so that we can control the horizontal divergence in the velocity increments.
  - Improve assimilation of high-frequency ageostrophic component (e.g. near-inertial oscillations), e.g. "rotated IAU", 4DVar.
- Improve *model representation* of the momentum coupling between the ocean, waves and atmosphere.
- Given large impact of assimilating these simulated velocity data, now working on global assimilation of surface-drifter derived velocity data.
- Should we call for an increase in surface drifter network to improve sampling of velocities and support satellite missions?











## 2. Ongoing developments and future directions

2.1 Observing systems

2.2 Ocean and coupled modelling

2.3 Ocean and coupled data assimilation

2.4 The role of machine learning & digital twins

## 2.2 Ocean and coupled modelling – improving processes in N. Atlantic through grid refinements (AGRIF)

#### Mixed Layer Depth



Labrador Sea dynamics: <u>local mesh refinement (1/20°)</u> for better resolving <u>mesoscale activity</u>, <u>mixed layer depth and overturning</u> in the Labrador Sea.





Nordic Sea overflows: <u>local terrain following</u> <u>coordinates</u> to better resolve <u>dense water</u> <u>cascading</u> (results in a better lower limb of the AMOC).

Bruciaferri et al., 2024

#### Absolute Sal. bias (model-obs) @ 550 m





Mediterranean overflow: <u>local mesh refinement (1/20°)</u> <u>combined with local terrain following coordinates</u> to improve the Med overflow and mesoscale dynamics, <u>significantly reducing the strong salinity biases in</u> <u>the North Atlantic</u>.

**Gulf Stream dynamics:** <u>local refinement of the mesh</u> for a <u>more realistic Gulf Stream separation</u> and mesoscale dynamics.





### 2.2 Ocean and coupled modelling – stochastic schemes



Storto & Andriopoulos, 2021, QJRMS



- SPPT: Stochastically perturbed parametrization tendencies
- SPP: Stochastically perturbed parameters
- SKEB: Stochastic Kinetic Energy Backscatter scheme





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## 2.2 Ocean and coupled modelling – land-sea coupling

Decrease of MAE in the Tropical Atlantic Ocean by using a gravimetry-derived estimate of the Amazon river runoff (using a mass balance approach), being further improved through the use of ML-based bias correction of hydrological models (projects WAMBOR, F3O of the Copernicus Marine Service).



**Bias Salinity** 



Mitigation of salinity bias (against independent in-situ) using interactive river runoff in a regional ESM NEMO+WRF+HD



**Pioneering Research** 













## 2. Ongoing developments and future directions

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#### 2.3 Ocean and coupled data assimilation

Some examples of ongoing areas of developments:

- Representing spatially correlated observation errors in variational DA.
- Ensemble and hybrid data assimilation.
- Coupled data assimilation.

Many other areas of development not covered here, e.g.

- $\circ$  4DVar
- High resolution and multi-resolution DA
- o Improved methods for reanalysis (e.g. bias correction, simplified smoothers)





#### 2.3 Ocean and coupled data assimilation – observation error correlations

Correlation functions modelled with diffusion on observation mesh





#### Accounting for correlated observation error in variational DA

Method:

- Observation locations used to define a *finite element mesh*;
- **Diffusion operator** used to model the spatial correlations on that mesh.

Impact:

- Ignoring correlations in observation errors can lead to an analysis worse than the background;
- Observation error variance inflation can be used to avoid this degradation but severely limits the positive impact of the observations;
- Accurately representing the observation error correlations in the DA reduces the analysis RMSE compared to optimal variance inflation;
- Accounting for observation error correlations improves the retrieval of small scales features from the observations.



Goux, Weaver, Piacentini.





• In data assimilation, the background error covariance matrix, *B*, determines how information from the observations is weighted and spread (horizontally, vertically and between variables).

• Difficult to estimate **B** due to its dimension (O( $10^{19}$ ) elements for global forecasting system at  $1/12^{\circ}$  resolution).

In variational methods, *B* is usually modelled using a combination of statistical estimates from previous reanalysis, parameterisations, and physically-based balance relationships.
=> Disadvantage is the lack of information about the "errors-of-the-day".

In ensemble methods, *B* is estimated using an ensemble of model states
=> Disadvantage is that limited ensemble size results in sampling noise (spurious correlations).

• Hybrid methods combine the static information from existing **B** models together with the ensemble information from an ensemble of the day.

SST ensemble spread



SSS ensemble spread









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60

40

20

-20

SST



Met Office global 1/4° FOAM ensemble (36 members):

model perturbations, ensemble inflation (RTPS)

0

Ensemble atmospheric forcing, EDA with obs perturbations, stochastic

Increments S/N cross-section in Gulf Stream (2018/09/01) => Ensemble gives more dynamically consistent structures



Latitude



Change in RMSE of the ensemble mean for SLA  $\beta_{e}^{2}$ =0.8 vs pure 3DVar

Future direction:

-60

-120

-0.100 -0.075 -0.050 -0.025 0.000

Implementing these ensemble developments in  $1/12^{\circ}$  global system.

180

Implementation in coupled NWP ensemble

60

0.025

120

0.050 0.075 0.100







- Impact of hybrid DA in the ECMWF ensemble ORAS6 system (11 members) using NEMOVAR software.
- ORAS6 uses the ensemble to determine both the climatological errors and the errors-of-the-day to adjust the parameters in an existing parameterised **B** matrix (rather than use the localised ensemble covariances directly).



Impact on the SSH innovations standard deviation. The errors are plotted relative to those of the baseline experiments, which used a parameterised **B**.



Globally averaged normalised RMS T profile errors. The baseline experiment with the parameterised **B** marks the 100% line.



Chrust et al., 2024





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#### **Operational Global Ensemble Kalman Filter**

- EnKF-C software. 1/10° resolution system.
- Deterministic ensemble transform KF. Asynchronous ensemble KF.
- Hybrid ensemble Kalman Filter
  - 48 dynamic ensemble members
  - 144 stationary ensemble members representing low modes
  - Inflation factor (3%)
- Localisation radius (T,S,SLA,SST)≡(450,450,175,150) km

 $\mathbf{P}^f = \partial \mathbf{P}^{dyn} + \partial \mathbf{P}^{stat}$ 

 $a = 1.03 \quad g = 0.25$ 

Summary of improvements

Reduction in increment variance

Reduction in abyssal KE noise

Improved separation of eddies

Improved skill of ocean currents

Reduced forecast error growth

Forecasts beating persistence

More dynamically balanced increments

Sustaining low signal to noise eddies

Reduced fictitious baroclinic instability

#### 40°N 0° 20°S 40°S 40°S 40°S 60°S 0.15 0.11 0.15 0.11 0.15 0.11 0.15 0.11 0.07 0.15 0.11 0.07 0.03 increme 0.07 0.03 RMS(En RMS(En



The Bureau of Meteorology



Pavel Sakov, Gary Brassington, Prasanth Divakaran, Matthew Chamberlain, Saima Aijaz, Jessica Sweeney, Xinmei Huang, Stewart Allen



Brassington et al., 2023 Chamberlain et al., 2021 Sakov and Oke, 2008 Sakov et al., 2010 Sakov, 2014







### 2.3 Ocean and coupled data assimilation – coupled error covariances

- Frolov et al. 2021 used the NRL global coupled ensemble to assess the nature of the atmosphere/ocean error covariances.
- Wright et al., 2024 followed this up using the Met Office coupled ensemble to assess how variable these covariances are.
- The 44-member coupled ensemble includes the ocean ensemble developments mentioned earlier, has a 6-hour cycle, with weakly coupled DA (atmosphere/land/ocean/sea ice).
- Cross-correlations vary diurnally, from day to day, spatially and synoptically.
  - Significant positive correlations of SST with 10 m wind speed in mid-latitudes are synoptically dependent and tend to be associated with areas of stronger winds.
  - They extend vertically into the ocean, throughout the mixed layer, which can be quite deep in these situations
  - Negative correlations between SST and 10 m wind speed in tropical oceans associated with warm SST and low wind speeds.









Wright et al., 2024





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### 2.3 Ocean and coupled data assimilation – coupled error covariances

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- The 44-member coupled ensemble includes the ocean ensemble developments mentioned earlier, has a 6-hour cycle, with weakly coupled DA (atmosphere/land/ocean/sea ice).
- Cross-correlations vary diurnally, from day to day, spatially and synoptically.
  - Negative correlations between SST and 10 m wind speed in the tropics associated with warm SST and low wind speeds.
  - These were linked to diurnal variations in solar radiation, with correlations strengthening as the ocean surface heated throughout the day.
  - These correlations were in locations of shallow mixed layers and remained at the surface.









Correlations between SST error and 10 m wind speed error as a function of the validity time of the six-hourly forecast on December 15, 2019.



Wright et al., 2024



-0.5

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### 2.3 Ocean and coupled data assimilation – coupled ocean/atmosphere DA

#### **Future directions**

- Using flow-dependent correlations, e.g. from coupled ensembles, will be key to the effectiveness of strongly coupled DA.
- Differing vertical extents of the correlations imply that the length scales used in the vertical localisation of ensemble correlations would need to be situation dependent.
  - => Methods such as those described by Stanley et al. 2024 could be used.



- Various other ways to increase the coupling in the DA (see e.g. de Rosnay et al, 2022) including:
  - coupled observation operators,
  - outer loop coupling,
  - coupled 4DVar with coupled tangent linear/adjoint models.
- Implementation of strongly coupled DA requires a *common software infrastructure* for the DA in the different earth system components, e.g. JEDI, ...













## 2. Ongoing developments and future directions

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## Soft use of machine learning/AI

VS

## Hard use of machine learning/AI







(Heimbach et al., 2024)

Augmenting current systems with AI elements (soft use of AI)

Learning (and correcting) systematic state-dependent errors in the air-sea heat fluxes through AI, with neural networks trained on SST assimilation increments over well-observed periods.

Application: reanalyses (early periods) and forecasts

From Storto et al., 2024 (in review for GMD).

#### **Bias-correction**



#### SST Forecasts (Global Ocean)



#### SST Forecasts (Tropics 30°S–30°N)







Ocean Predict

Augmenting current systems with AI elements (soft use of AI)

Observation and balance operators

NN-based OO for acoustic data assimilation in ocean models (from Storto et al., 2021)

Avoiding the use of complex and strongly nonlinear observation operators

(promising also for balance operators)

Dcean



NN-based OO for radiance data assimilation in atmospheric models (from Liang et al., 2023)

Towards a radiative transfer model-free assimilation of satellite data

(promising for assimilation of L1 data)





Augmenting current systems with AI elements (soft use of AI) Model parametrizations



$$\mathbf{S}^{\uparrow} = \left( \overline{\mathbf{u}^{\uparrow}} \cdot \nabla \right) \overline{\mathbf{u}^{\uparrow}} - \overline{\left( \mathbf{u}^{\uparrow} \cdot \nabla \right) \mathbf{u}^{\uparrow}}$$

Subgrid forcing term Learnt using CNN architecture from filtered and coarsegrained 1/10° resolution model simulations (CM2.6)

from Guillaumin & Zanna, 2021 JAMES; see also Perezhogin et al., 2023

Specifically for the NEMO model, we have a Working Group on Machine Learning and Uncertainty Quantification, to address technically online inference (and training) challenges, either through Fortran-linkable libraries or OASIS-callable python interfaces (see e.g. CNR/ISMAR ANNIF library; ECMWF Infero library; CNRS/IGE/MEOM EOPHIS package)





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Substituting (part of) current systems with AI elements (hard use of AI)



(from Barthélémy et al., 2024)

Full-physics or hybrid emulators?End-to-end ML for forecasting? Importance of conventional DA $\widehat{\mathbb{V}}$  $\widehat{\mathbb{V}}$ 

Re-thinking/Re-coding the ocean numerical models for AI and new HPC architectures



Julia-based model Oceananigans developed by Climate Modeling Alliance, CalTech, Silvestri et al., 2023







#### Digital twin for monitoring harmful blooms

In a previous project (CAMPUS) a digital twin was developed to track the onset of phytoplankton blooms (Ford et al., 2022)



#### SyncED-Ocean improvements

- Higher resolution (1.5km) operational coupled physics-BGC model
- Multiple gliders tracking multiple features
- Mutual cross-calibration of observational data-sets



3 gliders deployed Aug-Sep 2024 tracking Chl maxima, oxygen minima and gradient features



The 1.5 km model includes BGC DA (gliders and satellite) in a real time forecasting set-up.

Gliders are directed by a stochastic prediction model. The analysis of metrics evaluating the mission is on-going.



Skakala et al.









Lonesco
Karagespring
Commission



## **3. Summary and conclusions**

#### Conclusions

Much progress is being made in observing, modelling, data assimilation to address user needs:

- $\circ$  Improvements in observing systems, DA methods and modelling to improve accuracy
- Increases in model and DA resolution to resolve features of interest, even in the absence of constraining observational networks
- Development of ensembles to provide forecast uncertainty information
- $_{\odot}$  Coupled modelling and DA to produce consistent earth system prediction
- These areas are now being augmented by AI/ML methods, which in turn help reduce the misalignment of analysis and forecast tools with state-of-the-science computational paradigms.



CP-TT meeting Room III – Tomorrow 12:45









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Thank you!







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