Marine data assimilation in the UK: the past, the present and the vision for the future

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Abstract.

In the last two decades UK research institutes have led a wide range of developments in marine data assimilation (MDA), covering areas from operational applications in physics and biogeochemistry, to fundamental theory. We highlight the emergence of strong collaboration in the UK MDA community over this period and the increasing unification of its tools. We focus on identifying the MDA stakeholder community and current/future areas of impact, as well as current trends and future opportunities. This includes rapid growth of machine learning (ML) / artificial intelligence (AI) and digital twin applications. We articulate a vision for the future, including the needs for future types of observational data (whether planned missions, or hypothetical) and how the community should respond to increases in computational power and new computer architectures (e.g. exascale computing). We contrast the needs of different MDA areas, including physics, biogeochemistry and coupled DA. Although the specifics of the vision depend on each area, common themes emerge. We advocate for balanced redistribution of new computational capability among increased model resolution, model complexity, more sophisticated DA

algorithms and uncertainty representation (e.g. ensembles). We also advocate for integrated approaches, such as strongly coupled DA (ocean/atmosphere, physics/biogeochemistry, ocean/sea ice) and the use of ML/AI components (e.g. for multivariate increment balancing, bias-correction, model emulation, observation re-gridding, or fusion).

1 Introduction

Marine Data Assimilation (MDA) is the process of combining observations and model information to produce an estimate of the state of the ocean. Such estimates can provide a view of the history of the ocean (reanalysis), or provide the best available initial conditions from which predictions can be made. MDA is therefore a pillar of a "predictable ocean", one of the major challenges addressed by the United Nations (UN) Decade of Ocean Science for Sustainable Development (2021-2030) (https://oceandecade.org/). At the same time, ocean reanalyses are essential benchmarks for climate studies and are used to assess trends in the state of the ocean and derived services. Furthermore, since data assimilation (DA) is a tool at the interface of modelling and observation, it can provide essential information across the disciplinary boundaries, such as informing observational scientists on observing network design, or modellers on how to improve model configurations, forcing and parameterisations.

The UK plays a leading role in the international MDA community, hosting, or partly hosting, two major operational forecasting centres: the Met Office and the European Centre for Medium-range Weather Forecasts (ECMWF). The UK also has a strong reputation in DA theory, e.g. provided by the Data Assimilation Research Centre (DARC) of the University of Reading. The influence of the UK community extends internationally through organizations such as OceanPredict (including being instrumental in setting up the OceanPredict Data Assimilation Task Team and contributing to other Task Teams), its strong participation in expert groups (e.g. Mercator Ocean International DA expert group with impact on the Copernicus Marine Service) and through a range of international collaborations, such as the Met Office Unified Model (UM) Partnership, and a wide range of European Union (EU) Horizon and European Space Agency (ESA) projects. UK MDA is also a critical part of systems used to generate ocean products exploited for national and international marine policy and services, including the UN Sustainable Development Goals, the EU Marine Strategy Framework Directive, Blue Growth, marine safety, and national security (e.g. underwater operations).

UK MDA is a closely collaborating community with the collaboration largely facilitated by the UK National Partnership for Ocean Prediction (NPOP) and its MDA group. The role of this paper prepared by the NPOP MDA group is to both highlight the history of the ever-increasing collaboration within the UK community and formulate a unified vision for future developments. Whilst the paper is UK-focused, it should also be of interest to the broader international community, since it provides both a useful example of a successful national collaboration, and the UK vision will feed into international MDA developments due to the UK's leading role in this area. Furthermore, such focus allows topics to be explored with greater detail and synergy, complementing relatively recent international community reviews (e.g. Moore et al., 2019; Fennel et al.,

2019, Martin et al, 2025), as well as going beyond by discussing topics that emerged since some of those reviews were written. In this paper we first provide an overview of the main contributors to UK MDA and how they collaborate, together with a range of stakeholder applications. Then we review developments of MDA in the UK in the last two decades, highlighting the increase in collaboration and convergence of tools. Furthermore, we provide a unifying vision for the near and longer-term future. The vision also reflects upon new, or currently accelerating areas, such as machine learning (ML)/ artificial intelligence (AI) and digital twins of the ocean[1], that could be combined with MDA for a substantial mutual benefit. Finally, a vision is formulated for the infrastructure providing the resources for MDA, such as ocean observations, computer software and hardware, and people.

2 The UK MDA community and its stakeholders/beneficiaries

The UK MDA community includes DA scientists, as well as ocean modelling and observational scientists providing inputs to MDA development. The UK Institutes which directly contributed to MDA developments in the recent history are shown in Fig.1. These institutions interact closely through NPOP and its MDA Activity Group, with NPOP providing also broader interaction with other model developers and observational scientists. These include Institutes such as Centre for Environment, Fisheries and Aquaculture (Cefas) and Marine Directorate. Some of the MDA partners also interact through the National Centre for Earth Observation (NCEO), with NCEO providing additional links to the broader environmental (e.g., atmospheric, terrestrial) community. The areas of expertise of each MDA institution from Fig.1 are listed in Table 1. Fig.2 provides a simplified flow-diagram of collaboration for the main UK Institutes currently developing and running MDA software.

[1] Digital twins are understood here in a quite specific sense, as systems interacting two-way (exchanging information both-ways) with the twinned physical object, whilst operating as a real time decision-making tool. The fully autonomous observing systems described here fullfil this operational definition of digital twin.

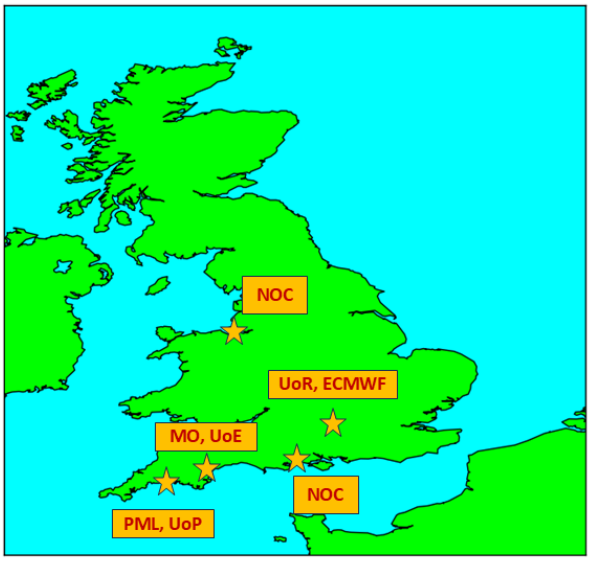

Fig.1: *The UK institutions directly contributing to UK MDA developments in the recent history. The abbreviations are: University of Plymouth (UoP), Plymouth Marine Laboratory (PML), Met Office (MO), University of Exeter (UoE), University of Reading (UoR), European Centre for Medium-Range Weather Forecasts (ECMWF), National Oceanography Centre (NOC). The PML and University of Reading research is also done and funded as part of the NCEO. It should be emphasized that ECMWF is a European institution rather than a UK one, but is partly based in the UK and has significant impact on UK MDA.*

Table 1: *The UK institutions with major past and present involvement in UK MDA and their areas of expertise. The orange color marks past-only contributions to the specific area, the dark color marks both past and ongoing present contributions to the area. The Table marks the situation as of 2025.*

Institute	Physical model development	Physical DA	Biogeochemistry model development	Biogeochemistry DA	Coupled DA	DA theory	Observations
ECMWF	✓	✓			✓	✓	✓
Met Office	✓	✓		✓	✓	✓	✓

NOC	✓	✓	✓	✓			✓
PML			✓	✓	✓		✓
University of Exeter				✓			✓
University of Plymouth		✓				✓	
University of Reading	✓	✓		✓	✓	✓	✓

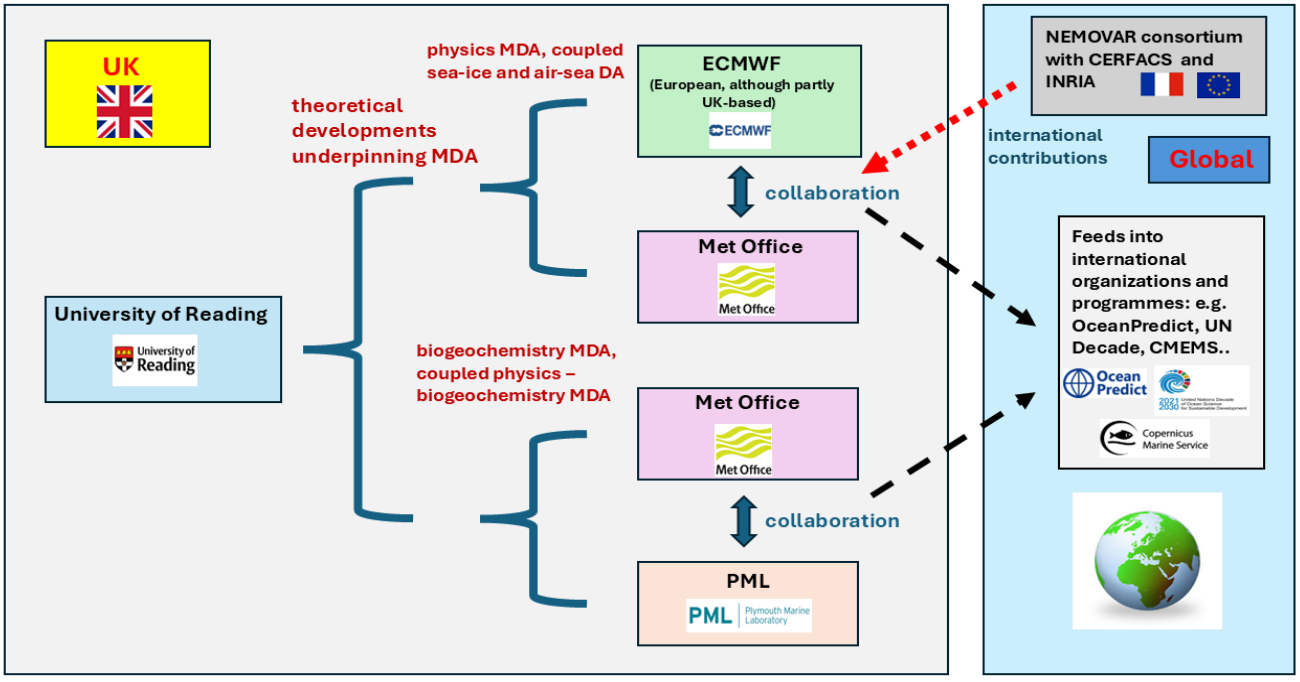

Fig.2 *A simplified diagram showing the main lines of collaboration between the largest UK Institutes currently involved in developing and running MDA software. The blue lines indicate the collaborative workflow, with University of Reading providing theoretical underpinnings for many developments across all MDA areas, which are split into two groups: (i) physical, coupled air-sea and sea-ice MDA developed in collaborative efforts involving the Met Office and ECMWF, and (ii) biogeochemistry and coupled physics-biogeochemistry MDA developed largely in collaboration involving the Met Office and PML. There is also a wider international input into the physics DA collaboration from the NEMOVAR consortium involving Centre Européen de Recherche et de Formation Avancée en Calcul Scientifique (CERFACS) and Institut national*

de recherche en sciences et technologies du numérique (INRIA). Other used abbreviations are: Copernicus Marine Environmental Monitoring Service (CMEMS).

UK MDA supports a wide range of stakeholder applications across the public and private sectors. It contributes to operational forecasts and reanalyses of key marine variables, both globally and regionally with higher fidelity, as well as to underlying scientific research. Key stakeholder applications of UK MDA are split below into end-user and scientific applications.

2.1 End-user applications

Real-time forecasts, initialised using MDA, are produced each day with various time ranges from a few hours to seasons ahead. Reanalyses are also produced which give information about the past state of the ocean. Ocean physics, sea ice, biogeochemistry, surface waves and weather information are all made available routinely to both specific users and the wider public. Existing and potential applications include:

- marine environment monitoring and prediction. This is of interest to national government departments (e.g. Department for Environment, Food & Rural Affairs) and agencies (e.g. Environment Agency), local councils, and industries including aquaculture and fisheries. Uses include the assessment of risk and planning the response to extreme events such as hypoxia, harmful algal blooms, and marine heatwaves. Products providing information about water quality and ocean health are also used, as are longer-term climate projections. Examples include spatial maps of oxygen deficient areas from Ciavatta et al (2016), which were included in an OSPAR assessment report on good environmental status (*https://oap.ospar.org/en/ospar-assessments/quality-status-reports/*), and analysis of trends in marine heatwaves by Berthou et al (2024).
- marine safety and offshore industry (including energy and net zero) applications, such as beach safety, safe and efficient ship navigation, design and operation of offshore oil, gas and renewables, including providing ambient water characteristics for management of import/export capacity for UK energy sources using underwater cables and pipelines. Examples include work by Stephens et al (2018) and Copernicus products, such as *https://marine.copernicus.eu/services/use-cases/safe-transport-gas-north-sea*.
- coastal flooding forecasts to help prevent loss of life and infrastructure/property damage.
- near-real time products for national defence applications derived from variables including temperature, salinity, currents, and visibility.
- marine accident response including search and rescue applications, and marine pollution incident response. Examples include pollution tracking systems run by Cefas using ocean currents from regional analyses and forecasts (*https://www.cefas.co.uk/science/emergency-response/)*.

- climate change projections contributing to the IPCC reports. UK MDA already contributes to initialization of such projections, but could in the future improve climate projections through better model parameter estimates, since a traceable set of models is jointly used for short-range forecasts, seasonal predictions and climate projections (e.g. Storkey et al., 2018).
- coupled ocean/atmosphere weather forecasts at short-range and seasonal timescales, and at global and regional scales. This includes forecasting events such as storms over the UK and Europe, tropical cyclones, monsoons, and El Niño events (Guiavarc'h et al, 2019).
- a range of very high-resolution coastal ocean operational systems, such as West of Scotland Coastal Ocean Modelling System (WeStCOMS, https://www.sams.ac.uk/facilities/thredds/) and Western Channel Observatory Operational Forecast (WCOOF) take boundary conditions from ocean analysis and forecast products. These can then feed into downstream systems such as HAB Reports (Davidson et al., 2021).

2.2 Scientific applications

As well as the users described in the previous section, there are both existing and potential scientific uses of products generated through MDA in the UK, and the UK MDA systems themselves:

- use of reanalysis products to understand and monitor key climate metrics such as the variability and trends of the Atlantic Meridional Overturning Circulation, sea ice extent and volume, and ocean heat, salt and carbon content. This includes reanalyses of ocean health indicators, such as pH to monitor ocean acidification, dissolved oxygen to identify trends in hypoxia, and net primary production to monitor biological productivity changes. Examples are decadal analyses of fluxes and indicators, including the phytoplankton community, in the UK regional seas (Ciavatta et al, 2016, 2018; Clark et al., 2020), as well as eco-regions and carbon fluxes in the Mediterranean Sea (Ciavatta et al, 2019).
- reanalyses are used to initialize future projections by the ocean and climate modelling community (including the coastal modelling community) and as lateral boundary conditions to drive smaller-scale, regional models (Ciavatta et al, 2016, McLachlan et al, 2015, Tinker and Hermanson, 2021, Polton et al, 2022). Data generated by those projections then benefit the whole scientific community.
- realism and full data-coverage of reanalyses, as well as improved parameters and process estimates generated by MDA, support the community studying ocean processes (including scientific hypotheses testing) and metrics. Examples include improved understanding of North Atlantic circulation in Jackson et al. (2019). An interesting example inspiring future work can be a paper by Cole et al, (2012), who used reanalysis (however, produced by non-UK institutes) to identify the impact of missing data on phenology metrics calculated from ocean colour observations.

- reanalyses are also being used in the context of machine learning (ML) model development, where they have the advantage of providing gap-free structured training data (constrained by observations), instead of the intermittent observational products. Examples include emulators predicting marine oxygen (Skakala et al, 2023a) and an ML model predicting marine nitrate (Banerjee and Skakala, 2024), both on the North-West European Shelf (NWES).
- improving model parameters using joint parameter-state estimation. This could feed into improved physical and biogeochemical (BGC) short-range, seasonal and climate projections, as well as underlying research applications. Examples include using 1D frameworks for parameter estimation such as the Marine Model Optimization Testbed (Hemmings et al, 2015) and the Ensemble and Assimilation Tool (Bruggeman et al, 2024), or estimating growth and mortality parameter variations in simple BGC models (Roy et al., 2012).
- reanalyses are a source of information on model performance and biases, which has led to a series of reanalysis intercomparison projects feeding into both model and DA development (e.g. Balmaseda et al, 2015).
- MDA can also support sensitivity studies and help identify essential drivers behind specific processes. Examples include comparing the relative sensitivities of carbon flux estimates with respect to model configurations and assimilated variables at L4 station in the western English Channel (Torres et al, 2020).
- the products generated using MDA are underpinned by good observing systems. Making best use of the existing and past observing systems is one of the main motivations for the development of MDA methodology. This includes demonstrating impact of existing observations through Observing System Experiments (OSEs), sometimes referred to as data denial experiments (Eyre, 2021), in which different combinations of observation types are assimilated to assess the impact of including or withholding certain observation types on model analyses and forecasts. Examples include OSEs applied globally to a range of physical observational types (Lea et al, 2014), including Argo (King et al, 2020), satellite sea surface salinity (Martin et al, 2020), satellite sea ice thickness (Mignac et al, 2022), different ocean color products (Ford and Barciela, 2017) and combined physics and biogeochemistry observations (Ford, 2020).
- observational array design can be influenced through Observing System Simulation Experiments (OSSEs). Examples include Mao et al. (2019) who participated in multi-system global OSSEs (Gasparin et al., 2019) assessing possible changes to Argo and moored buoy arrays, Ford (2021) who assessed the impact of assimilating different distributions of BGC-Argo floats, and King and Martin (2021) who ran regional OSSEs to assess the assimilation of wide-swath altimetry observations from the Surface Water and Ocean Topography (SWOT) mission. Some recommendations can be based on alternative methodologies using MDA, one of them using information cross-entropy was recently presented in Skakala et al, (2024).
- MDA can be used for a range of other observational applications, e.g. to improve satellite retrieval algorithms, especially in optically complex waters, navigate fully autonomous platforms into regions of observational interest (a digital twin reducing cost and carbon footprint), contribute to detection of problems with observing systems in real

time using automatic statistical quality control techniques, and investigate consistency between different observational products. Examples include navigating gliders to track the onset of phytoplankton blooms in Ford et al, (2022), Partridge et al, (2025) in prep, and exploring consistency of different satellite data types in Ford (2020).

- reanalysis data can be used for interpreting drivers of change seen in biodiversity datasets, such as from the Continuous Plankton Recorder, e.g. see the work of Holland et al., (2024). Looking more into the future, reanalyses have also the potential to assist with interpreting newer, rapidly growing datasets including those based on environmental DNA (eDNA).

3. The areas of UK MDA

In this section we review the history and the current state within different UK MDA areas. We highlight both the work done at different UK Institutes and the collaborative efforts across the Institutes, as well as internationally. As shown by the diagram in Fig.2, many of the key theoretical developments underpinning UK MDA are concentrated at DARC, based at the University of Reading, and are then advanced into MDA applications in collaboration with partners such as the Met Office, ECMWF and PML. It should be noted that similar transfer of theory developed at DARC is happening in wider UK environmental science, where fundamental DA theoretical developments are an underpinning theme to the research activities of NCEO, which seeks to advance the use of satellite data for understanding the carbon, water, and energy cycles.

There are many examples of theoretical results that have been transferred to MDA applications, most of them based on joint work of DARC with other UK partners. Examples include:

- developments in forecast and observation error covariance estimation used within marine biogeochemistry DA (Fowler et al, 2022),
- ongoing work on coupling systems, e.g. on improved estimation and treatment of in-domain and cross-domain covariances in the coupled air-sea DA system run at the Met Office (e.g. Leung et al, 2022, Wright et al, 2024),
- non-linear DA algorithms (e.g. the development of parametric-free methods; Hu and van Leeuwen, 2021), which have been applied in marine biogeochemistry through a joint PhD studentship with PML,
- development of simplified methods for smoothers applied to Met Office reanalysis (Dong et al. 2021, 2023),
- bias-correction of model and observations, e.g. through development of VarBC theory and techniques applied at the Met Office (Francis et al., 2023, While and Martin, 2019),
- development of an ML-based balancing scheme in marine biogeochemistry through a joint DARC-PML studentship (Higgs et al, 2025),
- a new technique for dealing with different timescales in coupled systems, developed at the University of Reading, and being tested at the Met Office,

- developments in Parallel Data Assimilation Framework (PDAF, Nerger and Hiller, 2014) at the University of Reading applied with PML to assimilate carbon from space into a global marine biogeochemistry model,
- a nested method of DA developed and applied at the University of Plymouth (Shapiro et al, 2022, 2023), which employs an intermediate coarse model assimilating temperature, salinity and velocity in 3D, which then constrain a separate fine resolution model by assimilating the balanced physical data provided by the coarser model outputs.

There are also a number of other recent UK-based theoretical developments that have the potential to be transferred to UK MDA applications in the near future. These include reconditioning and preconditioning to improve convergence (e.g. Tabeart et al, 2020; Daužickaitė et al, 2021), metrics of observation impact (e.g. Fowler et al, 2020), theoretical work led by Imperial College on neural assimilation (Arcucci et al, 2020), important theoretical research on combining ML with DA with contribution from University of Reading (Bocquet et al 2019, Brajard et al 2020a,b), work done at ECMWF on model bias-correction in the context of the 4DVar (Bonavita and Laloyaux, 2020, Farchi et al. 2021).

In the following sections we will focus on how different developments are influencing the state-of-the-art across a range of topical MDA areas.

3.1 Physical ocean and sea ice data assimilation

Physical MDA in the UK started through development of different systems at the Met Office and ECMWF, with the tools later converging, enabling closer collaboration between the two operational centres. The first MDA system developed at the Met Office was the Forecasting Ocean Assimilation Model (FOAM) system produced in 1997 (Bell et al., 2000). This used an assimilation scheme based on analysis correction (Lorenc et al., 1991; Martin et al., 2007). Simultaneously, an ocean analysis "System 1" (Alves et al., 2004) was developed at ECMWF, providing initial conditions only for the seasonal forecasting system (Stockdale et al, 1998). It was developed around the Hamburg Ocean Primitive Equation (HOPE, Wolff et al., 1997) model and employed an optimal interpolation (OI) scheme for assimilation of observations. The ECMWF system grew over subsequent years into a full 3D assimilation scheme, assimilating a range of data (temperature, salinity, altimetry) with applications including also monthly forecasts (Balmaseda 2005, Balmaseda et al, 2008, 2009).

Convergence of the MDA used at the two operational centres, Met Office and ECMWF, began when the Met Office adopted the Nucleus for European Modelling of the Ocean (NEMO) model around 2007 (Storkey et al., 2010) and the NEMOVAR data assimilation system (e.g. Mogensen et al, 2009) after 2011 (Waters et al., 2015), whilst the same systems were also adopted by ECMWF as part of their new NEMO based ocean reanalysis system (ORAS4, Balmaseda et al., 2013) that replaced HOPE. This was at ECMWF further upgraded (in 2016) to the currently used OCEAN5 reanalysis system, which is still based on NEMO and NEMOVAR (Zuo et al, 2015, 2017, 2019). The use of these community systems for the ocean model and data assimilation has facilitated significant collaboration among UK and European partners over this period.

Presently, in the UK physical ocean and sea ice data assimilation is primarily developed at the Met Office, ECMWF and the University of Reading, with the underpinning NEMOVAR assimilation code being developed jointly by an international consortium comprising the Met Office, ECMWF, CERFACS and INRIA. The developments in NEMOVAR-based physics DA are also used by other UK Institutes, such as the University of Plymouth (Shapiro et al, 2022, 2023). NEMOVAR ocean physics assimilation is employed at the Met Office and ECMWF as a multivariate incremental 3DVar-FGAT (First Guess at Appropriate Time) scheme. It uses physical balance relationships to transfer information between physical ocean variables (Weaver et al., 2005) and employs an implicit diffusion operator to efficiently model the spatial background error correlations (Weaver et al., 2016). It includes bias correction schemes for sea surface temperature (SST, While and Martin, 2019), temperature and salinity profiles (Balmaseda et al, 2007, 2013), and sea level anomaly (SLA) data (Lea et al., 2008). There were recently major new developments to NEMOVAR functionality through the implementation of capability to use hybrid ensemble/variational algorithms, including efficient methods for ensemble localisation. This functionality has been developed to increase flow-dependence within background error covariances to improve the quality of physics reanalyses and forecasts. It was applied in the Met Office global marine physics DA system where an ensemble forecasting capability was developed, and the impact of using the ensemble information in the background error covariances in a hybrid-3DEnVar scheme was tested (Lea et al., 2022). Similar hybrid methods are becoming part of the upcoming ECMWF reanalysis system ORAS6 (Zuo et al., 2024, see Fig.3). Finally, early versions of hybrid physics DA have now been developed for applications within the North-West European Shelf (NWES) forecasting system (Skakala et al, 2024).

Operational short-range NEMOVAR-based forecasting systems are run at the Met Office and ECMWF for the global ocean and sea ice. Furthermore, the Met Office also runs regional short-range forecasts for the NWES, using high-resolution (1.5 km) coupled ocean-wave models. Global reanalyses have also been produced by the Met Office and ECMWF, and regional reanalyses by the Met Office, for many years, e.g. in support of seasonal forecasting. The systems assimilate SST data from both in situ and satellite platforms, SLA data from satellite altimeters, sea ice concentration (SIC) data from satellites and in situ profiles of temperature and salinity from various platforms. A detailed overview of observations available to those systems as well as our current capacity to assimilate them is given in Tab.2.

Upcoming developments to NEMOVAR include a more efficient and up-to-date implementation of 4DVar capability (by INRIA). 4DVar is computationally expensive in the large model configurations used operationally and would have a significant maintenance overhead. However, it could bring significant improvements in performance, making better use of observations, providing improved temporal consistency of outputs, and reducing shock in the initialisation of forecasts, all of which are important aspects for most stakeholders. There is also work being undertaken in the NEMOVAR consortium aimed at developing capability to represent spatial correlations in the observation errors (Guillet et al., 2019) which allow more information to be extracted from high-resolution satellite data such as from SWOT. A studentship at the University of Reading

(with funding from the Met Office) has investigated the control variables used to represent the horizontal velocities in ocean data assimilation which should improve analyses of velocity, an important variable for many stakeholders.

Table 2: *The marine observational types available to physical, and coupled sea-ice DA. For each type we indicate whether the data are operationally assimilated, or there is existing DA capability in research mode, or they are not assimilated at all. We also add comments on issues associated with their assimilation.*

Variable	Satellite (surface)	In situ (profiles)	Issues/Comments
Temperature	Available for decades (e.g. O'Carroll et al, 2019) and operationally assimilated	Available from Argo floats, gliders, moorings, ships (XBTs and CTDs), instrumented marine mammals and other platforms (Roemmich et al, 2019, Davidson et al, 2019), operationally assimilated	Improvements in measurements of deep ocean temperatures (below 2000m depth) in western boundary currents and in marginal seas are being explored, the major area of weakness for the UK community being the poor sampling of sub-surface temperatures on the NWES and adjacent ocean boundaries
Salinity	Available since 2010 (e.g. Vinogradova et al, 2019), assimilation capability established in Martin et al, 2019	Available for many years from Argo floats, moorings, gliders and ships (e.g. Davidson et al, 2019), operationally assimilated	The quality of salinity in situ data can be sometimes less than that of temperature (due to drifts that can be difficult to detect in real time, fouling and inherent challenges). Satellite sea surface salinity accuracy is lower than in situ measurements (particularly at mid-to-high latitudes).
Sea surface height (SSH)	Available since 1993 (Le Traon et al, 2018) and operationally assimilated, capability to assimilate Surface Water and Ocean Topography (SWOT) data	Tide gauges available (Ponte et al, 2019), but not assimilated.	Recent sampling by altimeters has allowed reasonable initialisation of mesoscale structures in the deep ocean, but is not good enough to constrain some of the higher frequency processes of interest to many stakeholders on the NWES, e.g surges, tides. SWOT (Morrow et al, 2019) is expected to improve the situation since it resolves the SSH at high

	introduced in King et al (2021)		resolution within its swath, but the long repeat cycle of 21 days means that it is still not ideal for constraining all the scales we would wish.
Ocean currents (velocity)	Currently not available	From surface drifters drogued at about 15m depth (e.g. Rohrs et al, 2023), High Frequency (HF) radar measurements near some coasts, from Acoustic Doppler Current Profilers (ADCPs) and subsurface currents from Argo drifts, not routinely assimilated, but their assimilation is being currently assessed	Sub-surface currents from Argo are inaccurate and their assimilation has not been explored in the UK, ADCPs are sparse and often not sustained so their value for assimilation into operational systems is difficult to assess.
Sea ice variables	Sea ice concentration widely available for decades and operationally assimilated. Sea ice freeboard and thickness data available, their assimilation established in research mode (e.g. Fiedler et al, 2022, Mignac et al, 2022, Williams et al, 2023).	Very rare and not assimilated.	Very few in situ measurements available for sea ice thickness, although they are still useful for reanalysis and model/DA validation.

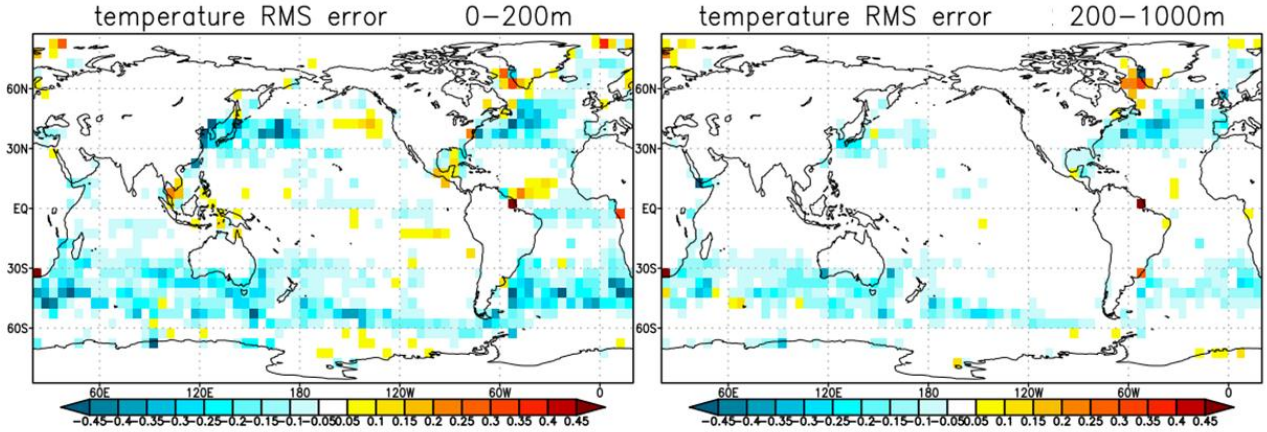

Fig.3. *Change in temperature Root Mean Square Errors (RMSE) between two experiments. The reference experiment uses parameterized background covariance matrix model, the second experiment uses the ensemble-based hybrid background covariance matrix model. Temperature RMSE is computed using model short-range forecasts against all in-situ observations in the upper 200 m (left) and in the 200-1000 m range (right), for year 2017. Negative values show improvement when using ensemble-based hybrid background covariance model.*

3.2 Biogeochemical (BGC) data assimilation

BGC DA research in the UK has mainly focused on state estimation, with some additional work on parameter estimation. Most past research on the latter took place at NOC prior to about 2013 (e.g. Fasham and Evans, 1995; Hemmings et al., 2003, 2004), with support from NCEO funding. This culminated in the development of the Marine Model Optimization Testbed, a state-of-the-art tool for parameter optimisation in a multi-site 1D framework (Hemmings et al., 2015).

For state estimation, similarly to the physics DA, two main strands of work have developed concurrently, starting to intertwine and converge in more recent years. At PML, assimilation was developed for the complex European Regional Seas Ecosystem Model (ERSEM, Butenschon et al, 2016), first in 1D (Allen et al, 2003, Torres et al., 2006), then for the western English Channel (Ciavatta et al., 2011) and the whole NWES (Ciavatta et al., 2016). This used an implementation of the ensemble Kalman Filter (EnKF), with 100 ensemble members allowing multivariate updates, and 3D studies assimilating different products from satellite ocean colour, such as total and size-class chlorophyll, and diffuse attenuation coefficients (Ciavatta et al., 2011, 2014, 2016, 2018).

Assimilation for the simpler Hadley Centre Ocean Carbon Cycle Model (Palmer and Totterdell, 2001) was developed by the Met Office and NOC, applied to the global ocean. A sophisticated “nitrogen balancing scheme” was developed to

provide multivariate updates to non-observed variables in a computationally efficient manner without ensembles (Hemmings et al., 2008). This was combined with an analysis correction scheme to allow assimilation of chlorophyll from ocean colour (Ford et al., 2012; Ford and Barciela, 2017), optionally used with weakly-coupled assimilation of physics data. In addition, a scheme was developed for assimilation of in situ pCO_2 data (While et al., 2012). These schemes have since been applied with 3DVar using the NEMOVAR assimilation framework (Ford, 2020) and in Ford (2021) they were applied with the Model for ecosystem dynamics, nutrient Utilisation, Sequestration and Acidification (MEDUSA, Yool et al, 2013). MEDUSA is the ocean BGC model used in the UK Earth System Model which contributes to the Coupled Model Intercomparison Project (Sellar et al., 2019), so the adoption of MEDUSA for reanalysis studies allows for greater synchronicity with UK climate research. Ford (2021) introduced assimilation of multivariate in situ profiles as might be obtained from BGC-Argo data in an observing system simulation experiment using synthetic profiles. The work has been extended in a collaboration between the Met Office and University of Exeter, assimilating a wide range of biogeochemical observations from various sources including satellites, ships, and BGC-Argo floats to investigate their individual and combined ability to constrain the model's biogeochemistry (an example of this is shown in Fig.4).

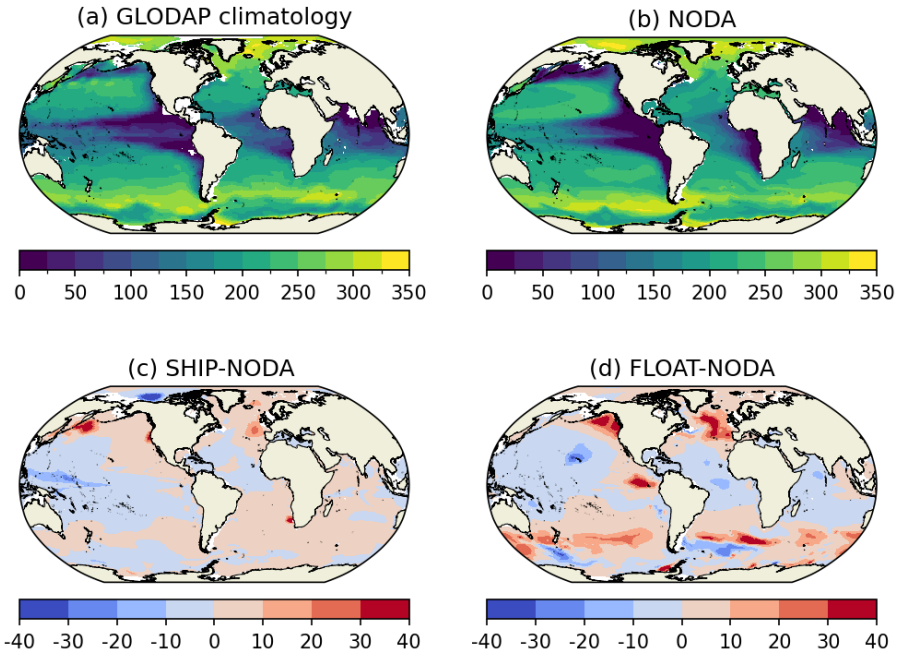

Fig. 4: *Impact of multi-platform BGC DA on oxygen (all in mmol/m3) at 200 m depth. (a) Oxygen concentration from the GLODAP climatology. (b) Oxygen concentration in December 2011 in a forced ocean-biogeochemical run, using NEMO-MEDUSA and forcing from ERA-Interim, without data assimilation (called "NODA"). NODA is initialised in 1980 from climatology (EN4 for temperature and salinity, GLODAP for biogeochemistry). (c) and (d) show the difference in oxygen*

concentration in December 2011 to NODA when assimilating biogeochemical data in 2011 only. (c) Assimilation experiment called "SHIP", using in situ biogeochemical observations from GLODAPv2022 (oxygen, dissolved inorganic carbon, alkalinity, pH, nitrate, silicate, chlorophyll) and SOCATv2022 (fCO2). (d) Assimilation experiment called "FLOAT", using observations from BGC-Argo floats (oxygen, pH, nitrate, and chlorophyll).

In more recent years the different MDA Institutes moved rapidly towards close collaboration in two different ways:

(i) The work at PML and the Met Office rapidly converged since 2016, when they started collaborating on development of BGC assimilation for the NWES using NEMOVAR and the 7 km resolution NEMO-FABM-ERSEM model. This was built on existing NEMOVAR-based physics assimilation and global BGC assimilation work at the Met Office, and was informed by the previous NWES BGC assimilation experience of PML. As in physics, the assimilation scheme is 3DVar, adding a basic balancing scheme for phytoplankton variables. The NWES operational forecasting system currently assimilates, alongside physics data, total chlorophyll from ocean colour (Skakala et al, 2018, McEwan et al, 2021). The NEMOVAR system was also used to provide a multi-decadal reanalysis for the Copernicus Marine Service (Kay et al, 2016), which included assimilation of size-class chlorophyll (Skakala et al, 2018). Further research activities involving collaboration between PML, Met Office and at several instances also the University of Reading, include introducing assimilation of novel satellite and in situ observational types in shelf seas (Skakala et al, 2020, 2021, 2022, Ford et al, 2022, for overview see Tab.3), improvement of the background error covariances for ocean colour DA using the diagnostic tools of Desroziers et al. (2005) (Fowler et al, 2022), and introducing fully flow-dependent background error covariances in the form of a 3DEnVar system (Skakala et al, 2024). There are several other ongoing developments within established collaborations including increasing the physics-biogeochemistry NWES model and assimilation resolution to 1.5km, to match the operational physics forecasting system (Tonani et al., 2019). This high-resolution BGC DA set-up was recently used in a digital twin mission tracking harmful algal blooms in the Western English Channel (Partridge et al, 2025, in prep, see also Fig.5). Another stream of work focuses on refining the ERSEM representation of optics by including explicit representation of colored dissolved organic matter, sediment, and their optical signatures. This latter work will also provide estimates of spectrally resolved reflectance for the NWES, and assimilate hyperspectral reflectance data into the model, further strengthening the link between our modelling efforts and the remote sensing algorithms of the Earth Observation (EO) community.

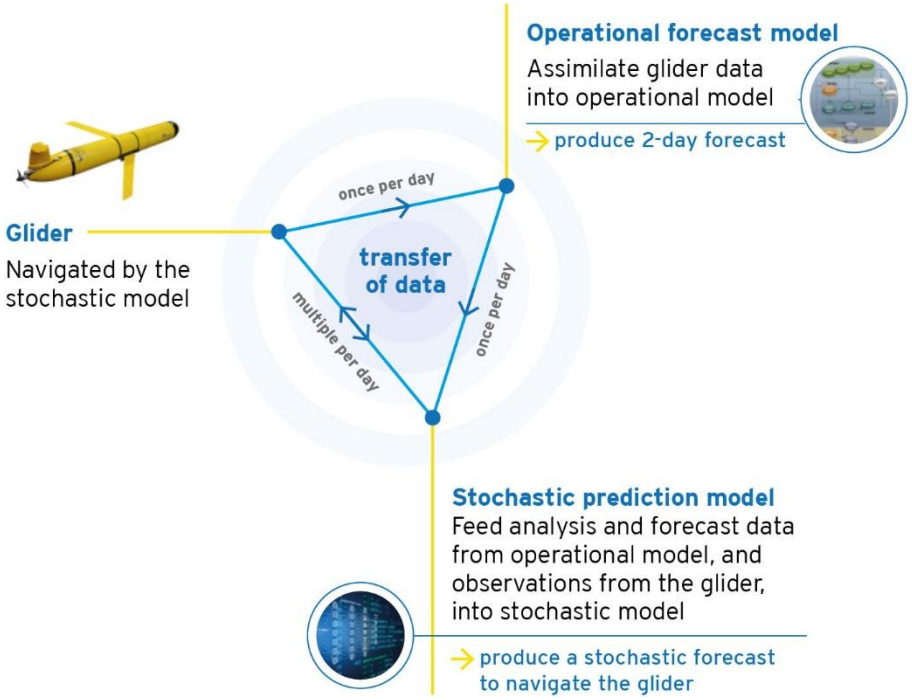

Fig.5. *A schematic illustration of a digital twin system navigating fully autonomous gliders to areas of observational interest. The Figure is reproduced from Ford et al (2022), with a similar scheme also being applied in Partridge et al (2025), in prep. The digital twin system is based on information flowing in all directions: (i) glider observations are being assimilated into the pre-operational forecasting model (i.e. the model is updated by the glider). (ii) The operational model subsequently produces forecasts for a stochastic/ML model, with additional inputs into the stochastic model provided by the glider directly, (iii) The stochastic model then provides the system with a fully autonomous path-planning capacity close to the glider's spatial scale of operations, navigating the glider into the expected areas of observational interest (i.e. the model tells glider "where to go"). This exchange of information then cycles throughout the glider mission.*

(ii) There is also a relatively new collaboration between University of Reading and PML implementing the Parallel Data Assimilation Framework (PDAF, Nerger and Hiller, 2013) for the global NEMO-MEDUSA model, mainly focusing on assimilation of carbon-from-space products. There is currently an effort to explore synergies with the global marine BGC DA products with the same NEMO-MEDUSA model at the Met Office and University of Exeter.

Table 3: *The marine observational types available to biogeochemistry DA. For each type we indicate whether the data are operationally assimilated, or there is existing DA capability in research mode, or they are not assimilated at all. We also add comments on issues associated with their assimilation.*

Variable	Satellite (surface)	In situ (profiles)	Issues/comments
Chlorophyll-a	Widely available derived from ocean colour since 1997 (e.g. Groom et al, 2019). Derived products splitting chlorophyll-a into phytoplankton size-classes have been developed, often tuned for a specific region (e.g. Brewin et al., 2017). Total and size class chlorophyll-a are operationally assimilated for forecasting and reanalysis respectively (Skakala et al, 2018).	Total chlorophyll available from buoys, gliders, BGC-Argo and ship measurements, the capability to assimilate those is established in research mode (e.g. Skakala et al, 2021, Ford et al, 2022)	Although the satellite data exist on fine spatial and temporal scales, they suffer from gaps due to cloudiness and low winter solar angle at high latitudes. Their accuracy and biases need to be better understood and accounted for in DA. In situ data are still quite sparse, but increasing in number, particularly with the spin-up of BGC-Argo and increasing use of gliders (Johnson and Claustre, 2016, Telszewski et al, 2018). Reconciling differences between in situ fluorescence and satellite ocean color remains a challenge.
Oxygen	Products using statistical/ML-based inference to derive oxygen from satellite observations of other variables exist (e.g. Sundararaman and Shanmugam, 2024), but are not assimilated.	Measurements from buoys, gliders, BGC-Argo and ships widely available. The capability to assimilate those has been developed and validated (Skakala et al, 2021).	Quality control of oxygen data remains a challenge for operational applications (e.g. Skakala et al, 2021)
Nutrients	Products exist which use statistical modelling/ML to derive nutrients from satellite observations of other variables (e.g. Chen et al, 2023, Banerjee and	In situ measurements of nitrate, phosphate, ammonium and silicate are made by buoys, gliders, BGC-Argo and ships (not all nutrients	In situ nutrient observations are sparse, especially in near-real time. The reliability of

	Skakala, 2024, Sundararaman and Shanmugam, 2024). Assimilation of such a product for nitrate has been developed and tested on the NWES (Banerjee et al, 2025, in prep).	available from all platforms). Some data are also derived from other variables through ML algorithms (Sauzede et al, 2017). Assimilation of nutrients has been established and tested in research mode (Ford, 2021).	ML/statistically-derived data needs to be better understood.
Carbonate variables	There are products which derive carbonate variables from satellite observations of other variables (Land et al, 2015, Shutler et al, 2024), but these are not assimilated.	There are rich data-sets for partial CO2 pressure (pCO2), or alternatively CO2 fugacity (fCO2), obtained from ships and moorings. Furthermore, BGC-Argo can include measurements of pH, and direct measurements for dissolved inorganic carbon and total alkalinity are available from ships. pCO2 assimilation has been developed in research mode (While et al, 2012), and assimilation of a wider range of carbonate variables has been recently established as well (e.g. Ford, 2021).	The carbonate data offer great potential for assimilation that has not been utilized to its full extent.
Other biogeo-chemistry variables	There is a relatively wide range of products derived from satellite ocean colour, including for phytoplankton carbon, net primary production, particulate organic carbon (POC, both detritus and living), remote sensing spectral reflectance, spectral diffuse attenuation coefficients (Kd), spectral phytoplankton size-class absorption and even some regional products for zooplankton carbon, or global ML-derived products for dissolved organic carbon (e.g. Groom et al, 2019, Kulk et al, 2020, Brewin et al, 2019, 2021, Laine et al,	BGC-Argo, buoys, ships, gliders and other in situ platforms can provide a range of variables, such as optical measurements, organic carbon pools and phytoplankton and zooplankton biomass. Furthermore, other types of data are becoming available, e.g. from omics, acoustics, plankton imagery. These data are presently not being assimilated.	The quality and reliability of these satellite-based products varies, but in some cases their assimilation might be taken to complement the more standard methods, such as chlorophyll DA (e.g. optical variables DA could have advantages over chlorophyll in turbid waters). Temporal resolution of some of the products might represent some challenges (e.g. phytoplankton carbon is produced with monthly resolution). In situ data are sparse

	2024, Kong et al, 2024). Assimilation of some of these products has been already established: i.e. of reflectance, Kd, by Ciavatta et al, (2014), phytoplankton size-class absorption in Skakala et al, (2020) and more recently also of satellite phytoplankton carbon.		and sometimes not easily matched to model state variables. So far, the preferred option has been to use them for model development, calibration and validation.

3.3 Coupled data assimilation

DA is often used in the context of coupled dynamics between different Earth System components, e.g. atmosphere and ocean physics, ocean physics and ice, or ocean physics and ocean biogeochemistry. The dynamical coupling between those components raises the question whether (i) separate DA solvers should be used for each component, with the assimilation increments from these separate DA systems being used to initialise a forecast of the coupled model, which is called "weakly" coupled DA, or (ii) the information about the coupling (e.g. cross-covariances) between the different components should be included into the DA system, which we call "strongly" coupled DA. The current state-of-the-art UK MDA systems are weakly coupled, but there is an overall drive towards introducing strong coupling.

Weakly coupled air-sea systems are part of ECMWF (de Rosnay et al, 2022) and Met Office (Lea et al, 2015, Guiavarc'h et al., 2019) operational short-range weather forecasts. The ocean part of the Met Office coupled NWP ensemble system is currently being developed to include improved ensemble forecast generation methods and the use of hybrid-3DEnVar (Lea et al., 2022; 2023). This will allow improved uncertainty propagation from the ocean to the atmosphere through the forecast, leading to improved forecast uncertainties in both ocean and atmosphere, and should also enable improvements in the accuracy of the ocean physical variables. It should be noted that a regional coupled ocean-atmosphere modelling framework has also been developed as a UK collaborative programme for Regional Environmental Prediction (Lewis et al., 2019) and the Met Office plans to move towards operational regional coupled predictions. Advances towards strongly coupled air-sea DA have been made at ECMWF in reanalyses, such as CERA and CERA-SAT (e.g. Schepers et al, 2018), and much work has been done at the University of Reading on strongly coupled DA algorithms in simplified coupled models (Smith et al., 2015, 2017, 2018, 2020, Fowler and Lawless, 2016). Collaboration between University of Reading and the Met Office has also developed some understanding of the nature of atmosphere-ocean error covariances from the coupled ensemble (Wright et al., 2024, see also Fig.5). These different efforts will underpin future collaborative pushes towards strongly coupled air-sea DA systems.

As in air-sea coupled DA, the standard physical-biogeochemical assimilation is weakly coupled. It also typically uses one-way coupling between physics and BGC models (no impact of simulated BGC state on physics). Combining physics DA and biogeochemistry is an open research problem for the international MDA community (e.g. Raghukumar et al., 2015; Park et al., 2018; Gasparin et al., 2021). The inclusion of physics DA can degrade BGC model fields especially in equatorial regions (e.g. Park et al., 2018, Gasparin et al., 2021), and can also have modestly detrimental impacts on simulated phytoplankton in the NWES model (Skakala et al, 2022). Assimilating BGC data can compensate for this impact on the assimilated variables (Skakala et al, 2022), but the current systems do not fix the underlying issues, meaning non-observed variables can still be degraded, and biases can reappear during the forecast period. The combined impact of physics and BGC DA is also likely to be dependent on the assimilation methodology (Nerger et al, 2023), for instance how alignment of fronts and other features is considered (Anderson et al., 2000; Yu et al., 2018), and how increments of different variables are projected onto different scales (Waters et al., 2017). Improvements have been relatively recently explored in both the global (e.g. Waters et al., 2017) and NWES system, where through collaboration involving PML and Met Office, a two-way physics-biogeochemistry coupling was included into the model (Skakala et al., 2022, see Fig.6). Despite the early challenges (e.g. Bertino et al, 2021), strong coupling is for us a natural future aspiration, as it has the potential to improve simulations by maximising the use of information and helping ensure physical-biogeochemical consistency (Anderson et al., 2000; Yu et al., 2018; Goodliff et al., 2019; Izett et al., 2023).

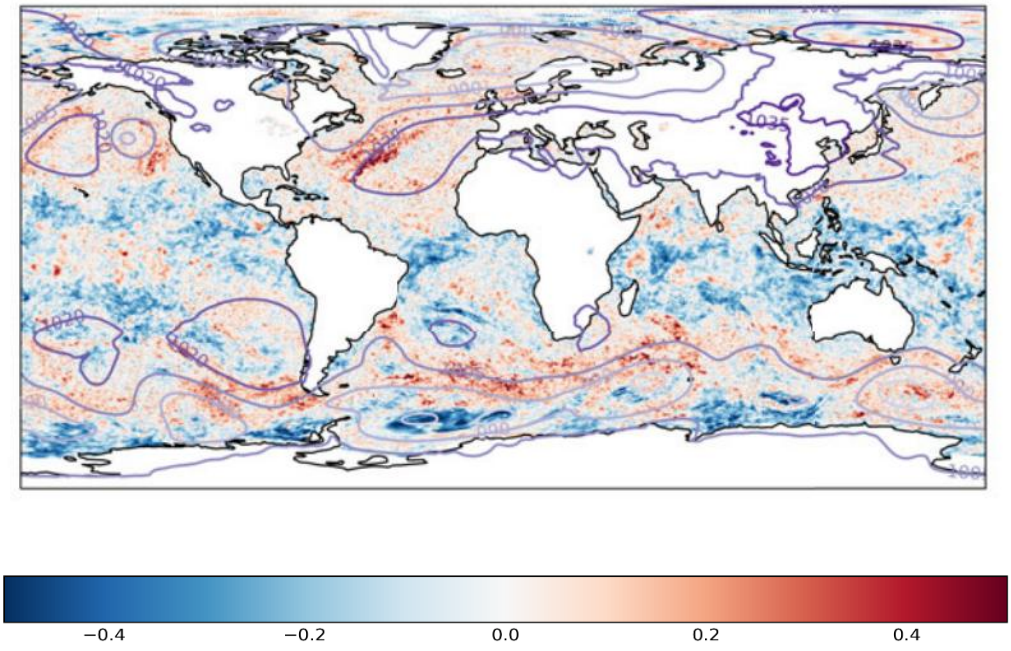

Fig.6. *Daily-mean correlations of sea-surface temperature and 10 m wind speed on December 5, 2019, with contour lines corresponding to the daily ensemble-mean sea-level atmospheric surface pressure field. The Figure is taken from Wright et al., (2024). In the tropics we see negative correlations associated with warm SST and low wind speeds, which are linked to diurnal variations in solar radiation, with correlations strengthening as the ocean surface warms throughout the day. In contrast, the significant positive correlations of SST with 10 m wind speed in the North Atlantic are linked with strong SST gradients and tend to be associated with areas of stronger winds, the location of which varies synoptically. These areas of larger ocean/atmosphere correlations in mid-latitudes were shown to extend vertically into the ocean, throughout the mixed layer (Wright et al., 2024).*

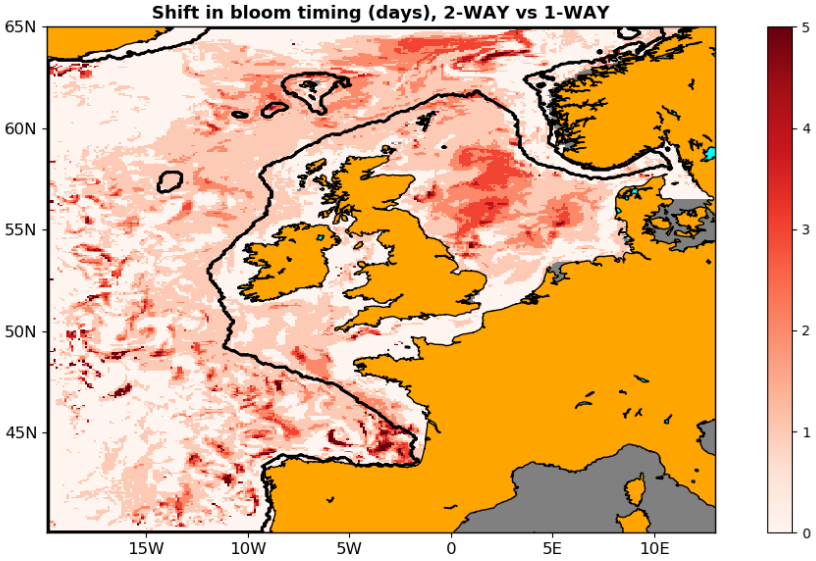

Fig.7: *Impact of two-way marine physics-biogeochemistry coupling on the timing of the phytoplankton spring bloom simulated by the NEMO-FABM-ERSEM model of the NWES. The one-way coupled model simulates late spring blooms, and the two-way coupling partly corrects this by moving the bloom timing earlier towards the start of the year. The Figure is taken from Skakala et al (2022) and shows the number of days by which the bloom timing shifts when the two-way coupling is introduced into the model.*

4. Vision for the future

4.1 Science

Different MDA areas have different needs and in this section we will contrast the differences and similarities in the future vision for those areas. Marine physics is typically more developed than marine biogeochemistry, uses better constrained models with fewer state variables (which often means lower model complexity), and has access to a greater abundance of observations with generally lower uncertainties and biases. Furthermore, marine biogeochemistry is much more strongly driven by marine physics than the other way round. Therefore, physics MDA developments are much more required for biogeochemistry than vice versa.

In the following sections we discuss the specific needs of each science area, followed by a section on needs that are common to all of them.

4.1.1 Physics MDA

Overall, the main future goal specific to the UK physics MDA is in resolving finer scale processes, both in space and time. There are a number of major goals that we envision:

We would like to build an efficient global ensemble hybrid 3DEnVar DA system at 1/12° spatial resolution (currently high-resolution forecasts are initialised using lower resolution DA). The global high-resolution ensemble system would improve forecasts for a range of stakeholders, including the navy, marine navigation, as well as better coupled numerical weather prediction and seasonal forecasting. Besides this common goal, there is also a specific Met Office goal to develop a shelf-seas ensemble hybrid-3DEnVar DA system at the 1.5 km resolution scale.

The high-resolution systems will be supported by the future capacity to assimilate new high-resolution observational types, such as SWOT wide-swath altimeter data to improve initialisation of mesoscale structures, high-frequency (HF) radar, Lagrangian drifter-derived velocities to improve velocity initialization and improved assimilation of sea ice thickness. A separate development supporting SWOT DA (and beyond) is to implement into NEMOVAR the capacity to deal with the observation error correlations, which could enhance the impact of fine-resolution observations.

Furthermore, quality of analyses of high frequency processes such as storm surges, tides and diurnal cycles, which are of interest to stakeholders near the coast, should be improved through the upcoming development of a NEMOVAR 4DVar capability. Such a system has particular use for the Met Office, where wave and storm surge forecasts are generated without any DA. Both waves and surge models are highly influenced by the wind (waves, surge) and atmospheric pressure (surge). Saulter et al. (2020) showed that assimilation of data into a regional wave model using NEMOVAR improved the forecasts over lead times of up to 12 hours, but errors in the surface forcing and wave model parameterisations dominated the forecast errors beyond 1-2 day lead time. We thus plan to develop capability to assimilate data within these forecasting systems to improve such shorter-range forecasts, and to improve the representation of the ocean/atmosphere interface when waves become integrated in Met Office operational coupled forecasting systems.

The main framework where all these physics MDA developments will be achieved will be NEMOVAR and should be based on the established collaboration between the University of Reading, Met Office and ECMWF, including additional

international partners of the NEMOVAR consortium. Most of these desired developments are underway, or are planned for the near future.

4.1.2 BGC MDA

Marine biogeochemistry models are less well constrained than their physics counterparts, with high uncertainties both in model formulation and their many parameter values. The complexity and non-linearity of marine BGC models, combined with the lack of routine observations of most state variables, puts high requirements on the methods used to update non-observed variables, be those balancing schemes or multivariate ensemble techniques. Furthermore, high model computational costs put substantial constraints on the use of ensembles. Therefore, BGC MDA developments often lag behind physics developments, and there are additional challenges associated.

An essential goal for BGC MDA is to develop more reliable multi-variate techniques. It is planned to assess both balancing and ensemble approaches, at first separately and then in combination. These can be based on the ensemble-NEMOVAR (3DEnVar) developments from Lea et al 2022 and Skakala et al 2024, through adapting and/or expanding existing balancing schemes (e.g. Hemmings et al, 2008), or using ML to learn relationships between observed and unobserved variables (as explored in Higgs et al, 2025). However, a number of hurdles leading to spurious cross-correlation estimates need to be bypassed, e.g. through expanding the range of perturbations used in the ensemble definition, or addressing systematic model biases (negatively impacting DA in general). The biases tend to be more significant in biogeochemistry than physics and tend to have their own seasonal signature (e.g. Skakala et al, 2018, 2022, Fowler et al 2022). Such biases could be corrected for example using ML, analogously to systems developed in the physical model domains (e.g. Bonavita and Laloyaux, 2020, for discussion see also Banerjee and Skakala, 2024).

Marine BGC also suffers from a lack of high-quality observations for many essential variables (e.g. carbon pools, nutrients, oxygen, pH). The situation is changing with new observational platforms like BGC-Argo and gliders, which can already be assimilated, and are starting to deliver a greater variety of BGC variables than are currently used operationally. It would be highly desirable to utilize such multivariate information and systematically assimilate these datasets. In situ BGC observations remain sparse though, and appropriate assimilation methods should be explored to maximise the information gained from these datasets, including historical ones. Similarly, multi-platform assimilation requires merging datasets across a wide range of spatial and temporal scales (including varying depths), and there is a lot of room to rethink and improve the algorithms that presently do so. Further advances in observation availability are expected through new hyperspectral satellite missions (e.g. PACE, Gorman et al, 2019), and those data should be harnessed for assimilation to a maximal possible degree. This includes improving the observation operators, through further refining the optical components of our models, and bringing the models closer to the water-leaving radiances seen by the satellites. Assimilation of reflectance data can also complement the traditional chlorophyll assimilation in optically complex waters, where remote sensing retrieval algorithms are less reliable. Improvements in optical components in our BGC models should also lead to these models/MDA becoming regularly used to inform EO retrieval algorithm developments.

Finally, BGC models do not sufficiently resolve the vast complexity of the real-world biogeochemistry, and have highly limited scope to account for biodiversity (using at best only a few "functional types" for plankton variables). These limitations could demonstrate themselves in spatio-temporal model parameter variability (e.g. Friedrichs et al, 2007), corresponding to the unresolved internal variability within the used functional types. The state estimation in our BGC DA systems should ideally be supplemented with estimation of BGC parameters, allowing for spatial and temporal variations in the parameter values. Spatio-temporally varying model parameter estimation may further improve model forecasts and contribute to better climate projections as well (e.g better constraining future net primary production projections).

Much of this work is either already being developed, has been funded, or is being currently incorporated in funding proposals. The stated goals will be pursued by the established collaboration between the University of Reading, PML and the Met Office, and based on (and around) NEMOVAR software, with some extra potential to further exploit PDAF (e.g. for parameter estimation) within the dedicated University of Reading and PML collaboration. There is also scope to more closely collaborate with the carbon and climate science communities, for instance building on existing collaborations with the University of Exeter.

4.1.3 Coupled MDA

The future focus and major challenge of the coupled DA is the advance to strong coupling. A key step advancing all strongly coupled systems is to explore the nature of error covariances across the coupled systems, using ensembles and a decision on how these should best be included in coupled DA algorithms. Additional challenges include the development of coupled observation operators to make use of data sensitive to both parts of the coupled system and the potentially different time-scales associated with different parts of the system (e.g. faster atmosphere dynamics vs slower ocean dynamics). Specifically, within the air-sea coupled DA, a closer collaboration between Met Office and ECMWF should be facilitated through using more common tools in the atmospheric domain (both centres use NEMOVAR in the ocean). These may be enabled by the Met Office atmospheric DA system moving to use the Joint Effort for Data Assimilation Integration (JEDI, with Lea and Martin, 2023, demonstrating the feasibility of ocean DA using NEMOVAR code in the JEDI). One of the JEDI tools is JEDI-Object Oriented Prediction System (OOPS), an assimilation control layer that is similar to OOPS which is used at ECMWF. Developments which implement coupled DA at this level are likely to be a collaborative effort. The community should in future be open to new methods to advance strongly coupled DA, such as those based on path signatures (Lyons, 2014) and signature kernels (Chevyrev & Oberhauser, 2018), which are designed to extract time-ordered moments from multivariate path data.

4.1.4 Topics common to the MDA areas

A common topic across the different areas is the need to address better model forecast uncertainty, i.e. in flow-dependent way. This need is also common to all the forecasting systems, whether global, or regional and is mirrored by the fact that all the operational systems envisioned by us involve the use of ensembles (e.g. 3DEnVar). The recently developed ensemble techniques representing model uncertainty (Lea et al, 2022, 2023, Skakala et al, 2024) should be further improved upon in the future, e.g. in terms of ensemble design. There are several options how to address the computational challenges associated with ensembles, including reducing the modelling cost through ML emulation (as discussed later in this section). The foundation for addressing this topic are the ongoing collaborations in this area involving University of Reading, Met Office, ECMWF and PML.

Furthermore, common challenges to the current reanalyses across different MDA areas are due to the changing observing systems over the reanalysis period, and due to responses of the model to the DA which sometimes introduces spurious signals that can contaminate the reanalysis products (e.g. spurious vertical velocities in the tropical regions). A range of model bias-correction techniques and data smoothing methodologies should be developed to improve the quality of ocean reanalyses, particularly in the period before Argo data are available, building on previous work by Zuo et al., (2019); Balmaseda et al. (2007); Bell et al., (2004) and Waters et al, (2017). This should allow more temporally consistent reanalyses to be produced, making them more suitable for climate and marine scientists studying past ocean changes. The current focus in this area is on ocean physics reanalyses, but smoothers could be equally used in marine BGC reanalyses. Furthermore, greater joint development of physical-biogeochemical reanalyses would benefit climate scientists studying the carbon cycle, such as those involved in the Global Carbon Budget (Friedlingstein et al., 2024). The proposed reanalysis research should build and expand upon existing long-standing relationships, such as those between the University of Reading, Met Office and ECMWF.

There are many new opportunities presented by the rapid development of ML/AI in DA and beyond (for a review of ML-DA methods see Cheng et al, 2023). DA can be thought of as a physically constrained ML framework (Abarbanel et al, 2018, Bocquet et al, 2020, Geer, 2021). This, and the wide range of potential ML applications (for oceanography see reviews by Lary et al 2018, Sonnewald et al 2021) make it very attractive to be aligned with DA. Hence ML, which has seen an explosion of research activities due to the rapid progress in high-performance computing (HPC) and increase in data availability, will be an increasingly present theme in research developments of DA. Future ML-DA work should include developing ML emulators that dynamically downscale coarser resolution models into higher resolution (e.g. for examples see Barthelemy et al, 2022), enabling us to emulate an ensemble of highly complex models (including applications in marine BGC) at very high spatial resolution at relatively low computational cost. Such emulators could then use DA to assimilate high resolution data, exploring also non-linear DA methods (this can be achieved for example through the use of PDAF). Other ML applications include emulating components of the physical model or the tangent linear model to improve the system's efficiency, emulating diffusion-based correlation matrix model, the (already discussed) model bias-correction (Farchi et al.,

2024) and learning, especially for biogeochemistry, balance relationships (Higgs et al, 2025). Furthermore, wherever costly ensemble DA systems are used, ML techniques could be developed to replace them with an emulator. Melinc and Zaplotnik (2023), developed 3DVar using a variational auto-encoder (VAE) where the minimisation is performed in a reduced-order latent space discovered by VAE and the background-error covariance matrix is learned from historical data. Approaches to emulate DA with ML can be possibly pushed further, as show the promising recent results by score-based data assimilation (Rozet and Louppe, 2023) and de-noising diffusion model data assimilation (Huang et al., 2024). We envision that all the future MDA systems used by the UK Institutes will be transformed via coupling with ML/AI components along these outlined examples. Work on this has already started, but should be accelerated through emerging funding opportunities and done in close partnerships with UK (and also international) centers of excellence for ML/AI in geoscience and DA applications, such as the University of Exeter, Imperial College, Alan Turing Institute and others. It will also be highly desirable to develop and improve ML/AI expertise within the MDA community itself, something that is already being addressed through dedicated training and skills exchange.

Finally, a very timely topic is the use of MDA within digital twins. The concept of digital twin has taken off in the international community, for example with the UN Decade Digital Twins of The Ocean (https://oceandecade.org/actions/-digital-twins-of-the-ocean-ditto/) programme and the European Digital Twin of the Ocean (https://www.mercator-ocean.eu/en/digital-twin-ocean/) led by Mercator Ocean International. The digital twin, as typically understood, is a system that in real time replicates the real environment, allowing information flow from the environment to the system and back, and enabling decision-making in real time (e.g. Blair, 2021). A nice example of such systems are fully autonomous observing systems (e.g. based on Autonomous Underwater Vehicles, AUVs, such as gliders) developed for purposes of tracking events and regions of observational interest. There is a very strong UK collaboration around the digital twin technology involving PML, Met Office, NOC and the University of Exeter, which has delivered examples of digital twins, based on one, or multiple, AUVs tracking observational events of interest, including inter-calibration of different observations (Ford et al, 2022, Partridge et al, 2025, in prep). MDA plays an integral role in such digital twins, as the AUVs are being navigated into areas of observational interest (see Fig.5) with the help of operational forecasts produced from an analysis state, in which the AUV's observations were assimilated into the model (Ford et al, 2022, Partridge et al, 2025, in prep). Such digital twin applications highlight further need of high-spatial model resolution (closer to AUV scales of operation), mostly within the coastal environment, and this should include marine biogeochemistry (Partridge et al, 2025, in prep). The biogeochemistry high-resolution models could cover large areas, such as the whole NWES (as Partridge et al, 2025, in prep), or could cover only smaller areas in the coastal zone. In such case they could be made relocatable, e.g. following techniques developed by Shapiro et al (2022, 2023). One of our priorities is that the marine digital twin developments accelerate in the future, serving the need of marine autonomy and net-zero science. A few issues will need to be addressed in the future, including (i) the high computational cost of modelling associated with high spatial resolution, and (ii) the digital twin being able to deliver target variables of interest (e.g. concentrations of harmful phytoplankton species), rather than what AUVs can typically measure (e.g.

fluorescence). We envision that ML/AI should help address both these issues, e.g. through providing cheap emulators for parts, or the whole high-resolution model, and adding digital twin components that could predict the target variables of interest from the observed/modelled variables. Furthermore, including more directly socio-economic data and modelling in the digital twin would be another desirable development. The future work on digital twins should be based on the established UK collaboration, but new partners should be brought in and stronger links to international digital twin activities should be developed.

4.2 Infrastructure

The critical infrastructure for MDA includes the models, observations, MDA software, hardware and people. Although marine model developments are essential to improve operational forecasts, they rarely expand the MDA capacity compared to, for example, new observation types. The few cases where we see potential for model advancement to improve MDA, such as refining our bio-optical models, have been noted in the previous section. The following sub-sections will focus only on the future vision for observations, MDA software, hardware and people.

4.2.1 Observations

A list of planned satellite missions for Earth Observation is available from the World Meteorological Organization (WMO) (https://space.oscar.wmo.int/satellites). Of particular interest to the UK MDA community are missions which will improve observations of sea ice thickness (CIMR, CRISTAL and ROSE-L), begin measuring surface ocean currents (Harmony, ODYSEA), increase the sampling of small-scale SSH features through wide-swath altimetry, following on from SWOT (Sentinel-3 next generation, COMPIRA), and provide continuity of existing measurements through the Sentinel programme.

Improvements to the Argo in situ network are also underway with the design of OneArgo focussing on three elements: improving the sampling by Argo in Polar sea ice zones and marginal seas; increasing resolution of Argo floats in the Western Boundary currents and equatorial regions; implementing more floats which measure biogeochemical variables (BGC-Argo) and which measure the deep ocean (Deep-Argo).

In terms of future need, the maintenance of the existing observing systems is still paramount, but areas that require urgent improvement to allow UK MDA systems to better meet stakeholder needs include: (i) improving the sampling of sub-surface temperature and salinity in the NWES region, (ii) improving measurements of surface currents both globally and around the coasts of the UK, (iii) improving in situ measurements of sea ice thickness to complement satellite data, (iv) increasing the number of observed essential BGC and bio-optical variables, as well as increasing the number of sub-surface observations, capturing biological features not seen from the satellites, such as deep chlorophyll maxima, (v) improving the accuracy and sampling of in situ measurements of the important BGC variables, alongside reliable uncertainty estimates, (vi) substantially increasing the number of coincident measurements of ocean and atmosphere, which could help assess the

estimates of cross-fluid covariances for strongly coupled DA, (vii) use of ML to develop more complete products derived from observations. Addressing this long list of requirements, however, necessitates new investment and approaches. One particular area we would like to highlight, particularly in the NWES environment, is autonomous ocean gliders. Gliders are increasingly being used to fill many of these requirements and have been demonstrated to work effectively in shallow shelf seas, filling a critical gap where Argo floats are largely ineffective. Gliders have the capability to provide sustained and regional scale (100s of km) measurements that cover almost the entire water column, from the surface to within a few metres of the seabed. Like many other marine science technologies however, gliders have mostly been deployed for short-term process studies, despite international efforts to coordinate and provide sustained capability (Testor et al, 2019). Gliders have however been shown to be cost effective for long-term multivariable monitoring of physical and biogeochemical states and change in UK seas (Loveday et al, 2022). Building on such demonstrators the Met Office invested in sustained operational deployments of ocean gliders in the North Sea from 2022, specifically targeted at improving sub-surface temperature and salinity on the NWES. The existence of such frameworks has the potential to provide a platform for further expansion of broad-scale, long-term monitoring of the NWES, helping to link up the variety of ongoing monitoring efforts from partner European states with autonomous mobile and adaptive measurement platforms. A number of research infrastructure initiatives have proposed frameworks around which to construct such coordination, including EU funded JERICO-RI and GROOMII programmes, but nothing yet exists to deliver funded, coordinated in situ monitoring of physical and biogeochemical states of the NWES.

4.2.2 MDA software

Traditionally a range of software was used within the UK MDA community, but the software use has now been largely unified around NEMOVAR. The software unification should be further continued by incorporating NEMOVAR modules into JEDI to support (collaborative) coupled air-sea DA developments. The focus on NEMOVAR as a unifying tool should be maintained, as this guarantees simpler pull through of methods to operational systems and makes better use of the limited human resources available. However, we recognise that there are some good reasons why fundamental research and operational applications might have different requirements from a software tool. Fundamental research needs ease of use and simplicity, while the operational applications need computational efficiency, robustness, and highly tuned configurations. This means full unification of DA software in the future is not expected. We will encourage the use of a single tool to allow for research pull through to operational systems and aim to move in this direction with the use of JEDI/NEMOVAR, but will keep the use of PDAF going for various important research applications (e.g. parameter estimation). Other software that has still been in use recently, such as PML EnKF (developed by Evensen, 2003, and adapted later for OC DA), might become less of a priority to maintain.

4.2.3 MDA hardware

UK MDA researchers have collective access to various high-performance computing (HPC) facilities including the NERC funded ARCHER2 facility and the Monsoon2 facility hosted at the Met Office. A Joint Ocean Data Assimilation Programme (JODAP) was implemented to make use of Monsoon2 HPC resources for various projects associated with the NPOP MDA activity group and associated PhD projects. This allows access to the Met Office's system for running research experiments for global and shelf-seas model configurations with both physics and BGC models and DA included. It has been used for numerous studies and has led to pull through of improvements in the DA applied to operational configurations.

Other facilities are also available for use in specific MDA Institutes, such as the PML hosted CETO and GPU MAGEO (which is also available more widely upon request) and clusters at universities. At the Met Office a new HPC is currently being installed which will provide a large increase in computing resources for research and operational uses, and ECMWF have very large HPC resources which can also be accessed for special research projects.

Over the next 5 years or so there will be increased access to machines which make use of GPUs, as well as the CPUs currently utilised by our research and operational MDA systems. Significant effort has been put in by the Met Office and others to allow the NEMO and NEMOVAR codes to be ported to GPUs and run efficiently on such machines. The approach has been to use the PSyclone software developed by the Science and Technology Facilities Council to parse the Fortran codes of NEMO and NEMOVAR in order to add directives to the code which allow the most computationally expensive regions to be run efficiently on GPUs. This separation of concerns means that the underlying Fortran code does not need to be changed (although some efficiencies to the codes have been identified through this process) and the use of the codes on different types of processors (CPU or mixed CPU/GPU) is separated from the scientific development of the code to a large extent.

For the future we recommend accelerating the capability of our MDA codes to run on GPU machines as well as improving the efficiency of the codes on large numbers of CPUs. We need to make sure we harness the increased computing power in the future by optimally distributing it into increasing resolution of the models, their complexity, sophistication of DA algorithms and the quality of ensembles/uncertainty representation. Finally, we will maintain and improve the ability to run operational configurations on research machines like Monsoon2 and its successors, so that researchers and PhD students outside the Met Office can run experiments with these realistic systems and improve the pull-through of developments into the operational systems.

4.2.4 People

The number of scientists working in MDA research and development is somewhat limited, and we need to keep bringing new scientists into the field as well as improving the training available to MDA scientists. There is a good availability of training activities across the community. ECMWF and DARC from the University of Reading run a coordinated set of annual introductory DA training courses (occasionally also offered under NCEO). There are also other courses on related topics (e.g. ensemble forecasting methods, satellite data assimilation) offered each year by ECMWF. Training is occasionally offered as

part of project dissemination, e.g. the EU Horizon project SEAMLESS developed a user-friendly DA software EAT for 1D "toy" models (Bruggeman et al, 2024) providing the opportunity for non-experts to develop practical DA skills. The University of Reading have recently developed a free Massively Open Online Course to introduce scientists to the basic ideas of DA and reanalysis (discoverda.org). Within the UK MDA community there is also a significant amount of PhD student supervision and often these are jointly supervised by different partners including PML, Met Office and the University of Reading. These activities help to bring in new scientists to the MDA field, as well as improving the collaboration between the different UK partners.

In the future we envision to develop and maintain people's skills through (i) joint student supervision, including improving the framework within which studentships are proposed, (ii) establishing opportunity for talented and motivated students to continue their career within the UK MDA community after completing their PhD, (iii) developing simple toy models and software tools (including their documentation) to enable the wider community to gain "hands-on" experience with MDA and (iv) upscale the existing MDA community in ML techniques and strengthen links with environmental ML centres of excellence.

5. Summary

Over recent years the UK MDA community has both substantially strengthened its collaboration and increasingly unified the diverse tools used at different institutes. It is therefore a natural point for the community to take stock of its achievements and outline its common vision for the future, which is the main purpose of this paper. In the vision we contrast the needs of different MDA areas ranging from physics to biogeochemistry to coupling multiple Earth system components. We formulate the future observational needs of MDA and a vision for the remaining infrastructure. Despite specific needs depending on individual subject areas, a common picture of the future emerges. This includes a rapid transition to ML/AI components playing a substantial role across all the MDA systems, enabling us to reach high resolution, realism and potentially even reduce the assumptions in MDA at an affordable computational cost. This should be further enhanced by exascale computing and use of GPUs. The variety of MDA applications should also increase, including underpinning the emerging concept of digital twins.

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